

Diffusivity in multiple scattering systems

Timothy Chumley*, Renato Feres*, Hong-Kun Zhang†

February 19, 2013

Abstract

We consider random flights of point particles inside n -dimensional channels of the form $\mathbb{R}^k \times \mathbb{B}^{n-k}$, where \mathbb{B}^{n-k} is a ball of radius r in dimension $n-k$. The particle velocities immediately after each collision with the boundary of the channel comprise a Markov chain with a transition probabilities operator P that is determined by a choice of (billiard-like) random mechanical model of the particle-surface interaction at the “microscopic” scale. Our central concern is the relationship between the scattering properties encoded in P and the constant of diffusivity of a Brownian motion obtained by an appropriate limit of the random flight in the channel. Markov operators obtained in this way are *natural* (definition below), which means, in particular, that (1) the (at the surface) Maxwell-Boltzmann velocity distribution with a given surface temperature, when the surface model contains moving parts, or (2) the so-called Knudsen cosine law, when this model is purely geometric, is the stationary distribution of P . We show by a suitable generalization of a central limit theorem of Kipnis and Varadhan how the diffusivity is expressed in terms of the spectrum of P and compute, in the case of 2-dimensional channels, the exact values of the diffusivity for a class of parametric microscopic surface models of the above geometric type (2).

1 INTRODUCTION AND GENERAL DEFINITIONS

We consider mathematical models of particle-surface systems involving multiple, or iterated, (classical) scattering. The purpose of this section is to motivate the main question regarding these systems and to introduce a few definitions needed to informally explain our results. More detailed statements will be given in the course of the paper.

1.1 AN IDEALIZED EXPERIMENT AND THE MAIN QUESTION

Figure 1.1 depicts an ideal experiment in which a small amount of gas composed of point-like, non-interacting masses is injected into a (for simplicity of exposition 2-dimensional) channel and the amount of outflowing gas per unit time is recorded. The graph on the right-hand side shows a typical exit flow curve. Possible gas transport characteristics that can be obtained from such an experiment are the mean value and higher moments of the molecular *time of escape*.

*Washington University, Department of Mathematics, Campus Box 1146, St. Louis, MO 63130

†Department of Mathematics and Statistics, University of Massachusetts, Amherst, MA 01003, USA

The central question then is: what can these time characteristics of the gas outflow tell us about the microscopic interaction (i.e., scattering properties) between gas molecules and the surface of the plates?

For a more precise formulation of this question, we begin by describing the classical surface scattering operators that model the microscopic collisions of the point mass. We refer to the boundary of the channel region as the (wall) *surface*, irrespective of its actual dimension.

Let \mathbb{H} denote the upper-half plane, consisting of vectors (v_1, v_2) with positive second component. Elements of \mathbb{H} represent velocities of a point mass immediately after a collision with the surface. By identifying $(v_1, -v_2)$ and (v_1, v_2) , we may regard pre-collision velocities as also being in \mathbb{H} . A *collision event* is then specified by a measurable map $v \in \mathbb{H} \mapsto \eta_v \in \mathcal{P}(\mathbb{H})$, where $\mathcal{P}(\mathbb{H})$ indicates the space of probability measures on the upper-half plane. The measurability condition is understood as follows: For every essentially bounded Borel measurable function ϕ on \mathbb{H} , the function

$$v \mapsto (P\phi)(v) := \int_{\mathbb{H}} \phi(u) d\eta_v(u)$$

is also measurable. We refer to P as the *collision operator*. This operator specifies the transition probabilities of Markov chains with state space \mathbb{H} giving the sequence of post-collision velocities from which the molecular random flight inside the channel can be obtained.

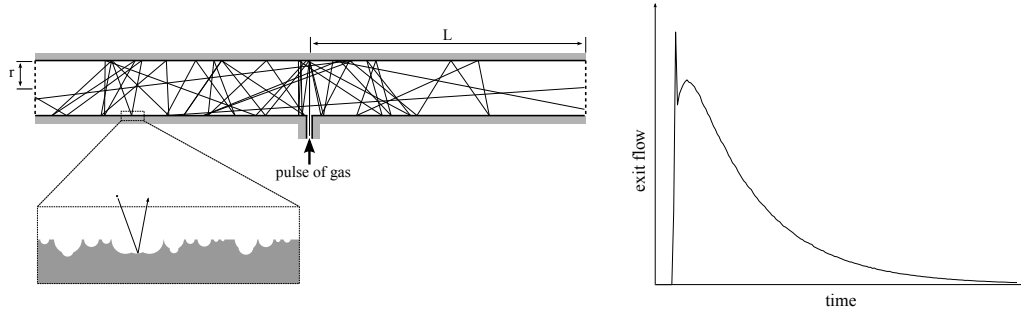


Figure 1.1: Idealized experiment in which a small pulse of gas is injected into a 2-dimensional channel and the gas outflow is recorded. The graph on the right represents the rate at which gas escapes. From this function it is possible to derive mean exit time of escape τ . The main problem is to relate easily measured properties of the gas outflow, such as τ , to the microscopic scattering characteristics of the channel surface.

If now $\tau = \tau(L, r, s)$ denotes the expected exit time of the random flight, where s is the molecular root-mean square velocity, then a more restricted form of the general question is to understand how τ depends on P . (This expected exit time is easily measured in actual experiments involving gas diffusion using the rate of gas outflow as represented on the right hand side of Figure 1.1; see, for example, [22] for so-called TAP-experiments in chemical kinetics.)

Although the analysis of P is generally simpler in dimension 2, an interesting complication arises here that is not present in the case of a 3-dimensional cylinder; namely, with respect

to the stationary distribution of velocities for natural collision operators (see the next subsection), molecular displacement between collisions has infinite variance and standard central limit theorems for Markov chains do not apply. The same is true for the random flight in the region $\mathbb{R}^2 \times [-r, r]$ between two parallel plates. In this regard, the random flight in a 3-dimensional cylindrical channel is simpler. (For an early study of two parallel plates case, see in [6].) Infinite variance of the in-between collisions displacements requires a generalization of the central limit theorem of Kipnis and Varadhan in [20] that is proved in this paper.

Now, from an appropriate central limit theorem we obtain for τ the asymptotic expression

$$(1.1) \quad \tau(L, r, s) \sim \frac{L^2}{\mathcal{D} \ln\left(\frac{L}{r}\right)}$$

for long channels in dimension 2, i.e., for large values of L/r , where $\mathcal{D} = \mathcal{D}(r, s)$ is the diffusivity of a limit Brownian motion. Therefore, a more specific formulation of the problem is to understand how properties of the collision operator are reflected on \mathcal{D} . A simple dimensional argument given in Subsection 2.2 shows that

$$\mathcal{D}(r, s) = \frac{4rs}{\pi} \eta,$$

where η only depends on the scattering characteristics at the microscopic scale determined by P . The choice of constants will become clear shortly.

The typical, but not the only type of operator we consider here is defined by a choice of microscopic contour of the channel wall surface, as suggested by Figure 1.1. The main problem then amounts to finding the functional dependence of η on geometric parameters of the surface microstructure. These parameters are scale invariant and are typically length ratios and angles. The presence of the logarithmic term in τ is related to some surprising properties of \mathcal{D} , as will be noted below, and for this reason we give somewhat greater prominence to the two-dimensional set-up in this paper.

1.2 NATURAL COLLISION OPERATORS AND MICROSTRUCTURES

Let $dV(v)$ denote the standard volume element on n -dimensional half-space $\mathbb{H} := \mathbb{H}^n$ and define the probability measure

$$d\mu_\beta(v) = 2\pi \left(\frac{\beta M}{2\pi} \right)^{\frac{n+1}{2}} \langle v, e_n \rangle \exp\left(-\frac{\beta M}{2} |v|^2\right) dV(v).$$

on \mathbb{H} . We refer to μ_β as the *surface Maxwellian*, or *surface Maxwell-Boltzmann distribution*, with parameter β and particle mass M . Here, $\langle v, e_n \rangle$ denotes the standard inner product (dot product) of $v \in \mathbb{H}^n$ and the unit normal vector, e_n , to the boundary surface at the origin. We often denote this normal vector by $n = e_n$. It will be clear in context whether n refers to dimension or to this normal vector.

In physics textbooks, $\beta = 1/\kappa T$, where T is absolute temperature and κ is the *Boltzmann constant*. A simple integral evaluation shows that the *mean squared post-collision speed* with respect to μ_β is

$$s_{ms}^2 := \int_{\mathbb{H}^n} |v|^2 d\mu_\beta(v) = \frac{n+1}{\beta M}.$$

Another distribution of collision velocities that arises naturally is concentrated on an hemisphere $S^+(s) := \{v \in \mathbb{H} : |v| = s\}$; it is defined by

$$d\mu(v) = \frac{\Gamma\left(\frac{n+1}{2}\right)}{s^n \pi^{\frac{n-1}{2}}} \langle v, n \rangle dV_{\text{sph}}(v)$$

where $dV_{\text{sph}}(v)$ is the volume element on the hemisphere of radius s induced from the ambient Euclidean space. In dimension 2, $d\mu(v) = \frac{1}{2s^2} \langle v, n \rangle dS(v)$, where dS indicates arclength element on $S^+(s)$. Equivalently, $d\mu(\theta) = \frac{1}{2} \cos\theta d\theta$, where θ is the angle between v and the normal vector n .

Definition 1 (Natural collision operators). *The collision operator P will be called natural if one of the following holds: (a) μ_β is the unique stationary distribution for P , for some β ; (b) the process defined by P does not change the particle speed and μ is a stationary probability measure for P for all s . If case (a) holds we say that the surface with associated operator P has temperature $T = 1/\kappa\beta$; in case (b) we say that P represents a random reflection. In addition, we demand in both cases that P and its stationary probability satisfy the detailed balance condition (see equation (20.5) of [23]). We use v throughout the paper to indicate either μ_β or μ .*

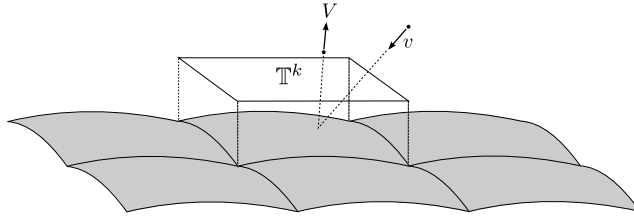


Figure 1.2: A periodic microstructure without moving parts. The cube containing a period of the microstructure defines a *cell*; the point in a k -dimensional torus \mathbb{T}^k at which the particle enters a typical cell is assumed to be a uniform random variable. The particle enters with pre-collision velocity v and exits with post-collision velocity V . The corresponding P describes a *random reflection*, as defined in the text.

The natural operators of particular interest to us are those defined by a choice of surface microscopic structure. We briefly described them here. (See [14], [15], [16], and [17] for more details.) By *surface (micro-)structure* we mean that the channel wall's surface has a periodic relief composed of *cells*, each consisting of a mechanical system of moving masses or more simply a fixed geometric shape with no moving parts. (Natural collision operators specified by the former correspond to part (a) of the definition, while the latter correspond to part (b).) Moreover, the wall system, mechanical or purely geometric, is assumed to be at a “microscopic” length scale that, by definition, is incommensurate with that of the channel defined, say, by the radius of the ball factor \mathbb{B}^{n-k} . At a collision event, the point particle enters a cell of the wall system, undergoes one or more deterministic collisions with it, transferring energy

between wall and particle in case (a), and leaves with a seemingly—from the perspective of the channel length scale—random velocity V . (See Figure 1.2.) Because of this assumption of incommensurability between the micro and macro scales, the relevant scattering properties specifying P are invariant under homotheties. Thus in dimension 2 we may, when convenient, assume that the width of each cell is 1.

This incommensurability also dictates our assumption that the particle position on the entrance of a cell at the beginning of a collision event is a uniformly distributed random variable. When the wall system has moving parts, the kinetic state of the cell at the moment the particle enters a cell is also drawn from a fixed probability distribution (a canonical Gibbs state at temperature T). Under these assumptions, V is an actual random variable and it can be shown (see [14]) that the associated collision operator P is natural according to Definition 1. The periodicity condition is not essential—all the basic facts discussed here hold, for example, for random structures, defined as probabilistic mixtures of periodic micro-structures.

The operator P can be expressed as follows. Let f be, say, a continuous bounded function on \mathbb{H} , and let V_+ be the random velocity immediately after the collision of a particle with incoming velocity $V_- = v$. Then

$$(Pf)(v) = \mathbb{E}[f(V_+) | V_- = v].$$

For example, in the purely geometric case of random reflections in dimension 2, P is given by

$$(Pf)(\theta) = \int_0^1 f(\Psi_\theta(r)) dr$$

where $\Psi_\theta(r)$ is the angle V makes with the normal vector n and $r \in [0, 1]$ is the position at which the particle enters a cell before collision. A similar integral over \mathbb{T}^k defines P in general dimension.

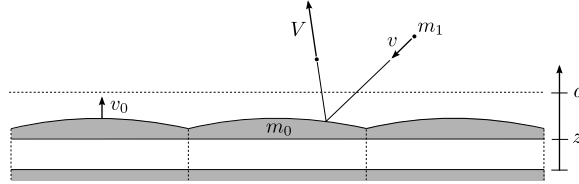


Figure 1.3: An example of a wall system with moving parts. Mass m_0 can move freely up and down, bouncing off elastically against the fixed floor and an upper limit that is permeable to m_1 .

Figure 1.3 illustrates a wall system with micro-structure having moving parts. The periodic relief is assigned a mass m_0 and can move vertically and freely over a short range of distances $[0, a]$ from the fixed base, bouncing off elastically at the lower and upper limits. The point particle of mass m_1 enters the wall system with velocity v at a uniformly random location along $[0, 1]$. Upon entrance, the velocity of the wall is assumed to be normally distributed with mean 0 and a given variance σ^2 , where $m_0\sigma^2$ is proportional to the wall temperature; the particle then goes on to interact deterministically with the wall, leaving with random velocity

V. This is a very special example of wall system for which P is natural. For other examples and details about random billiards with microstructures omitted here see [14]. See also [18] for a detailed analysis of this and other examples in the context of stochastic processes in velocity space \mathbb{H} having stationary measure μ_β or μ .

If we assume that the wall is static and has infinite mass, the system of the figure becomes purely geometric and the particle mass plays no role. In this case the operator P describes a random reflection. We refer to the subclass of natural operators derived from microscopic structures (either static or having moving parts, with arbitrary surface contours) as operators *associated to surface microstructures*. An interesting question suggested by [1] is whether general natural operators are limits of operators associated to surface microstructures.

Proposition 1. *The operators for the classes of examples of Figures 1.2 and 1.3 are natural.*

Proof. See [14, 18] for proofs of these basic issues related to stationary measures and more examples. \square

Occasionally, ν will stand for either of the two measures μ_β or μ of Definition 1. Because P and ν are assumed to satisfy the detailed balance condition, P is a self-adjoint operator of norm 1 on $L^2(\mathbb{H}, \nu)$. A further assumption for the main results below is that P be *quasi-compact*; that is, the spectral radius of P restricted to the orthogonal complement of the constant function in $L^2(\mathbb{H}, \nu)$ is strictly less than 1. Quasi-compactness for natural collision operators for the types of systems illustrated in Figure 1.2 is known to hold in a number of cases. The static version of the system of Figure 1.2 (for the specific shape shown in the figure) has this property (see [16], [17]), and the operator for the one-dimensional version of the moving wall is known to be compact (see [14]); the case of the two-dimensional moving wall is still open. Further examples of shapes of systems of the static type having quasi-compact P will be provided later in this paper.

Noting the two roles of P , as a self-adjoint operator on $L^2(\mathbb{H}, \nu)$ and as a Markov transition probabilities operator, a useful characterization of powers of P is as follows. Let V_0, V_1, \dots be a stationary Markov chain with transitions P and initial distribution ν and let $\Psi, \Phi \in L^2(\mathbb{H}, \nu)$. Then it is not difficult to show that

$$\langle \Psi, P^k \Phi \rangle = \mathbb{E}_\nu[\Psi(V_i) \Phi(V_{i+k})]$$

for any $i \geq 0$, where \mathbb{E}_ν indicates expectation given that V_0 is distributed according to ν .

2 RANDOM FLIGHT AND DIFFUSIVITY

2.1 BETWEEN-COLLISIONS DISPLACEMENTS AND TIMES

The logarithmic term in Equation 1.1 is a special feature of the random billiard process in regions bounded by parallel plates in arbitrary dimensions (in particular 2-dimensional channels bounded by a pair of parallel lines), and it is not present in the more typical cylindrical channel region $\mathbb{R}^k \times \mathbb{B}^{n-k}$ for $k = 1, \dots, n-2$. Ultimately, this is due to the mean square displacements being infinite in the two-plates case and finite in the other cases, as will be seen later. This elementary but key observation is highlighted in the next proposition.

Let $\mathcal{C} := \mathcal{C}^n := \mathbb{R}^k \times \mathbb{B}^{n-k}$ denote the channel region. Of special interest are the low dimensional cases: $n - k = 1$, for $n = 2, 3$ (two-dimensional channels and slabs in dimension 3) and $k = 1$, $n = 3$ (cylindrical channels in dimension 3). Let \mathbb{H}_q represent the upper-half space consisting of vectors $v \in T_q \mathcal{C}$, $q \in \partial \mathcal{C}$, such that $\langle n, v \rangle > 0$, where n is the unit vector in \mathbb{H}_q perpendicular to $\partial \mathcal{C}$ and $\langle \cdot, \cdot \rangle$ is the inner product given by restriction of the standard dot product in \mathbb{R}^n . If q' is the next collision point of the trajectory $t \mapsto q + tv$, let $Z(v)$ denote the natural projection to the “horizontal” factor \mathbb{R}^k of the vector $q' - q \in \mathbb{R}^n$. We refer to $Z(v)$ as the (*horizontal*) *displacement vector* for the given v . See Figure 2.1. The time of free flight between the collisions at q and q' will be indicated by $\tau_b(v)$.

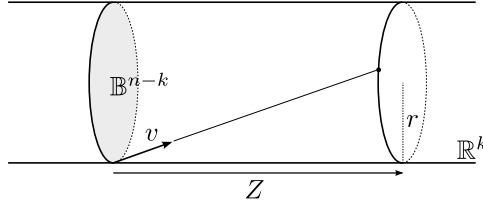


Figure 2.1: The between-collisions displacement vector $Z(v)$, where v is the post-collision velocity at a boundary point of the channel region. The time between two consecutive collisions is denoted in this section $\tau_b(v)$.

Proposition 2. *Let ν be either of the two probability measures of Definition 1 (denoted there μ_β and μ). This is a probability measure on $\mathbb{H} \cong T_q \mathcal{C}$ (concentrated on a hemisphere in the case of μ), for a given collision point $q \in \partial \mathcal{C}$. Let Z_a denote the product of Z and the indicator function of the cone $\mathbb{H}(a) := \{v \in \mathbb{H} : |Z(v)| \leq ar\}$ for $a > 0$. Also define for any unit vector $u \in \mathbb{R}^k$ the orthogonal projection $Z_a^u := \langle u, Z_a \rangle$. Then, if $n - k \geq 2$,*

$$\mathbb{E}_\nu \left[(Z^u)^2 \right] = \lim_{a \rightarrow \infty} \mathbb{E}_\nu \left[(Z_a^u)^2 \right] = \frac{4r^2}{(n-k)^2 - 1}.$$

If $n - k = 1$, then the asymptotic expression

$$\mathbb{E}_\nu \left[(Z_a^u)^2 \right] \sim 4r^2 \ln a$$

holds. The expected time of free flight τ_b (here ‘b’ is for ‘between collisions’) is finite for both types of measures and $n - k \geq 1$. For the stationary measure μ supported on the hemisphere of speed s ,

$$\mathbb{E}_\mu [\tau_b] = \frac{2r\sqrt{\pi}}{s(n-k)} \frac{\Gamma\left(\frac{n+1}{2}\right)}{\Gamma\left(\frac{n}{2}\right)}.$$

For μ_β , the corresponding expression is

$$\mathbb{E}_{\mu_\beta} [\tau_b] = \frac{r}{n-k} \sqrt{2\pi\beta M}$$

where M is particle mass.

For a sketch of the proof, see Section 5.1.

Before considering random flights in \mathcal{C} , we need to mention a technical point of geometric interest that only arises in dimensions $n > 3$, having to do with whether the operator P actually gives rise to a well-defined process in \mathcal{C} . The issue is that in order for a fixed P to induce a scattering operator at each $T_q\mathcal{C}$, $q \in \partial\mathcal{C}$, we need to be able to identify the positive part (say, inward pointing) of this tangent space with the half-space $\mathbb{H} = \{v \in \mathbb{R}^n : \langle v, e_n \rangle > 0\}$. Such identification amounts to specifying an orthonormal *frame* on the tangent space at each boundary point, which provides the information of how the model microstructure is “aligned” with the channel wall. Introducing a frame field on $\partial\mathcal{C}$ has, however, the effect that the scattering operator P_q at each boundary point q becomes a conjugate of P under an orthogonal transformation, rather than P itself. For all the cases in dimensions 2 and 3, namely $(n = 2, k = 1), (n = 3, k = 1), (n = 3, k = 2)$, there is a natural frame (the parallel transported frame over the boundary of the channel) with respect to which $P_q = P$ for all q . In the general case, $T_q\mathcal{C}$ has a canonical orthogonal decomposition into a “horizontal” part, naturally identified with \mathbb{R}^k , and a vertical part that splits orthogonally into the normal direction $\mathbb{R}n_q$ and the complement \mathbb{V}_q of dimension $n - k - 1$. We can now understand the issue as follows: Let v be a velocity vector of a particle that emerges from a collision at $q \in \partial\mathcal{C}$ and will collide again next at q' . In order that the Markov chain in velocity space be given by iterates of the same operator P , we need a field of orthonormal frames with respect to which v , at q , and its mirror reflection at q' have the same representation as vectors in \mathbb{R}^n . The components of these two vectors in \mathbb{V}_q^\perp and $\mathbb{V}_{q'}^\perp$, respectively, agree if we choose the canonical (parallel) frame, but on the subspaces \mathbb{V}_q themselves no such frame exists in general. With this in mind, and to avoid complicating the picture by introducing such frame fields as additional structure, we simply assume without further mention that P is \mathbb{V} -isotropic, that is, it is invariant under conjugation by orthogonal linear maps that restrict to the identity on $\mathbb{R}^k \oplus \mathbb{R}e_n$. Notice that this assumption is vacuous in dimensions 2 and 3.

2.2 DIFFUSIVITY, SPECTRUM AND MEAN EXIT TIME

Let \overline{X}_t , $t \geq 0$, be a piecewise linear path in the channel region \mathcal{C} describing a random flight governed by a natural collision operator P . Recall that P is a self-adjoint operator on $L^2(\mathbb{H}, \nu)$. We assume throughout that P is quasi-compact. (This is one of the conditions needed for Theorem 2, below.)

We wish to consider a diffusion process in \mathbb{R}^k obtained by an appropriate scaling limit of the projection of \overline{X}_t to the \mathbb{R}^k factor of \mathcal{C} . Let this projection be denoted X_t , and assume $X_0 = 0$. The sequence of post-collision velocities of \overline{X}_t is a stationary Markov chain V_0, V_1, \dots , with initial distribution ν . The displacement vectors, previously defined, are random variables Z_0, Z_1, \dots . Thus X_t , at collision times, are sums of the Z_i . The a -scaled random flight is defined as follows. Let $h(a)$, $a > 0$, be

$$h(a) = \begin{cases} a & \text{for } n - k \geq 2 \\ a/\log a & \text{for } n - k = 1. \end{cases}$$

Define the *scaled channel system* with scale parameter $a > 0$ to be the channel system with radius r/a and root-mean-square velocity $h(a)s_{ms}$. (If $\nu = \mu$, s_{ms} is the constant speed throughout the process and if $\nu = \mu_\beta$, $s_{ms}^2 = (n + 1)/\beta M$.) The random flight paths and their projection

are defined as the paths for the a -system. We denote them by $\overline{X}_{a,t}$ and $X_{a,t}$, respectively. The a -scaled free displacement with post-collision velocity vector v is $a^{-1}Z(v)$, and the displacements associated to the V_j are $a^{-1}Z_j$. For any $\tau > 0$, over a time interval $[0, \tau]$, the number of collisions of \overline{X}_t with $\partial\mathcal{C}$ will be written N_τ . For the a -scaled system this number is $N_{a,\tau} := N_{ah(a)\tau}$. For the cases in which $n - k = 1$, when $\mathbb{E}_v[|Z|^2]$ is infinite, it will be necessary to also consider the a -truncation Z_a of Z introduced above in Proposition 2. The a -scaled a -truncation of Z and Z_j will be written $a^{-1}Z_a$ and $a^{-1}Z_{a,j}$. Finally, we will like to follow the projected random flight along an axis set by a unit vector $u \in \mathbb{R}^k$. Thus we define Z^u , X_t^u , Z_a^u , etc., to be the orthogonal projections of Z , X_t , Z_a , etc., on $\mathbb{R}u$.

Theorem 1 below gives conditions under which $X_{a,t}$ converges to Brownian motion for large a . In this subsection, we wish to focus on the variance (or diffusivity) of the limit Brownian motion, and provide an interpretation of this constant in a way that does not make use of the physically somewhat artificial scaling just introduced. The precise conditions for the diffusion limit to exist when Z has infinite variance relative to v (i.e., for $n - k = 1$) are not yet fully clear; for Theorem 1 we make the following additional assumption that will be verified in the examples discussed later.

Assumption 1. Define for $\gamma > 1$ the set $\mathbb{H}^\gamma(a) := \{v \in \mathbb{H} : |Z^u(v)| \leq ar / \log^\gamma a\}$ and let $Z_{a,\gamma,j}^u$ be the product of Z_j^u by the indicator function of $\mathbb{H}^\gamma(a)$. Then, for any $t > 0$,

$$\lim_{a \rightarrow \infty} \mathbb{E}_v \left[\left(\frac{1}{a} \sum_{j=0}^{N_{a,t}} Z_{a,\gamma,j}^u \right)^2 \right]$$

exists for all unit vectors $u \in \mathbb{R}^k$.

This assumption, which will only be needed when $n - k = 1$, will be explained later in the context of Theorems 2 and 3. It is not needed for $n - k \geq 2$, when Z has finite variance and Theorem 1 is for the most part a consequence of well known limit theorems, in particular the central limit theorem for reversible Markov chains as formulated by Kipnis and Varadhan in [20].

Theorem 1 (Diffusion limit). *Let P be quasi-compact and, if $n - k = 1$, suppose that Assumption 1 holds. Then the a -scaled projected random path $X_{a,t}^u$, for a unit vector $u \in \mathbb{R}^k$, converges weakly as $a \rightarrow \infty$ to a Brownian motion in $\mathbb{R}u$ with diffusion constant \mathcal{D}^u further specified below. In particular, $X_{a,t}^u$ converges in distribution for each $t > 0$ to a normal random variable in $\mathbb{R}u$ with mean 0 and variance $t\mathcal{D}^u$. The following statements concerning \mathcal{D}^u also hold:*

1. *For the purpose of having a baseline value for \mathcal{D}^u , suppose that P maps probability measures to v . In other words, let the velocity process on \mathbb{H} be i.i.d. with probability measure v . Let $n - k \geq 2$. Then, denoting the constant \mathcal{D}_0^u in this special case,*

$$\mathcal{D}_0^u = \frac{4}{\sqrt{2\pi(n+1)}} \frac{n-k}{(n-k)^2 - 1} r s_{ms}$$

when $v = \mu_\beta$ and

$$\mathcal{D}_0^u = \frac{2}{\sqrt{\pi}} \frac{\Gamma(\frac{n}{2})}{\Gamma(\frac{n+1}{2})} \frac{n-k}{(n-k)^2 - 1} r s$$

when $v = \mu$. Recall that s_{ms} is the root-mean-square velocity for μ_β , and that μ is concentrated on the hemisphere of radius s in \mathbb{H} . Being independent of u , we denote these values by \mathcal{D}_0 .

2. For $n - k = 1$, the baseline diffusivities are

$$\mathcal{D}_0 = \frac{4}{\sqrt{2\pi(n+1)}} r s_{ms}$$

when $v = \mu_\beta$ and

$$\mathcal{D}_0 = \frac{2}{\sqrt{\pi}} \frac{\Gamma(\frac{n}{2})}{\Gamma(\frac{n+1}{2})} r s$$

when $v = \mu$, supported on the hemisphere of radius s .

3. The diffusion constant for a general P can now be written as $\mathcal{D}^u = \eta(u)\mathcal{D}_0$, where $\eta(u)$ has the following expression in terms of the spectrum of P . First consider the case $n - k \geq 2$ and define a probability measure on the spectrum by

$$\Pi^u(d\lambda) := \|Z^u\|^{-2} \langle Z^u, \Pi(d\lambda) Z^u \rangle,$$

where Π is projection-valued spectral measure associated to P and the inner product and norm are those of $L^2(\mathbb{H}, \nu)$. Then

$$(2.1) \quad \eta(u) = \int_{-1}^1 \frac{1+\lambda}{1-\lambda} \Pi^u(d\lambda).$$

Notice that $\eta(u)$ is quadratic in u . Now suppose $n - k = 1$ and define for each a the probability measure

$$\Pi_a^u(d\lambda) := \|Z_a^u\|^{-2} \langle Z_a^u, \Pi(d\lambda) Z_a^u \rangle$$

on the spectrum and the function $\eta_a(u) = \int_{-1}^1 \frac{1+\lambda}{1-\lambda} \Pi_a^u(d\lambda)$. Then the limit $\lim_{a \rightarrow \infty} \eta_a(u)$ exists and defines a quadratic function $\eta(u)$ of u .

Proof. The limit theorems in probability theory we require are standard in the case $n - k \geq 2$ and will be proved later for $n - k = 1$ in Theorems 2 and 3. Here we only indicate how \mathcal{D}_0 and the expression for $\eta(u)$ in terms of the spectrum of P are obtained.

Recall that $N_{a,t} = N_{ah(a)t}$ is the number of collisions of the a -scaled random flight with the boundary of the (a -scaled) channel region during time interval $[0, t]$. Let τ_j denote the time duration of the step with (non-scaled) displacement Z_j . Then, as

$$(\tau_0 + \cdots + \tau_{N_T-1})/N_T \leq T/N_T \leq (\tau_0 + \cdots + \tau_{N_T})/N_T$$

for any $T > 0$, we can apply Birkhoff's ergodic theorem to obtain $\mathbb{E}_\nu[\tau_b] = \lim_{T \rightarrow \infty} T/N_T$, where we have used a previous notation τ_b for the random time between consecutive collisions.

Although not necessary in this case, we use here the truncated displacement Z_a , so that the derivation of the spectral formula will also apply to the infinite variance case to be discussed later (under the more stringent conditions needed in that case). It will be shown later

in Proposition 7 that, for any $t > 0$,

$$(2.2) \quad \mathcal{D}^u = \lim_{a \rightarrow \infty} \frac{1}{a^2 t} \mathbb{E}_v \left[\left(\sum_{j=0}^{N_{a,t}-1} Z_{a,j}^u \right)^2 \right].$$

In the i.i.d. case, this gives

$$\mathcal{D}^u = \lim_{a \rightarrow \infty} \mathbb{E}_v \left[(Z_a^u)^2 \right] \frac{N_{a,t}}{a^2 t} = \lim_{a \rightarrow \infty} \frac{h(a)}{a} \mathbb{E}_v \left[(Z_a^u)^2 \right] \frac{N_{ah(a)t}}{ah(a)t} = \lim_{a \rightarrow \infty} \frac{h(a)}{a} \frac{\mathbb{E}_v \left[(Z_a^u)^2 \right]}{\mathbb{E}_v[\tau_b]}.$$

We can now invoke Proposition 2 to obtain the values claimed for \mathcal{D}^u in the i.i.d. case.

Next we obtain the spectral formula for $\eta(u)$, beginning from expression 2.2. This expression holds without further assumptions in the finite variance case, and it follows from Assumption 1 when $n - k = 1$ as will be shown later in Proposition 7. Because P has positive spectral gap and Z_a^u has zero mean, the measure Π has compact support in the interval $(-1, 1)$. In particular, $1 - \lambda$ is bounded away from zero on the support of $\langle Z_a^u, \Pi(d\lambda) Z_a^u \rangle$. Now observe that, for $j \geq i$,

$$\mathbb{E}_v \left[Z_{a,j}^u Z_{a,i}^u \right] = \langle Z_a^u, P^{j-i} Z_a^u \rangle = \int_{-1}^1 \lambda^{j-i} \|Z_a^u\|^2 \Pi_a^u(d\lambda).$$

With this in mind, we obtain for a fixed N after some algebraic manipulation,

$$\mathbb{E}_v \left[\left(\sum_{j=0}^{N-1} Z_{a,j}^u \right)^2 \right] = \int_{-1}^1 \left(N + 2 \sum_{j=1}^{N-1} \sum_{i=0}^{j-1} \lambda^{j-i} \right) \|Z_a^u\|^2 \Pi_a^u(d\lambda) = \int_{-1}^1 \frac{1+\lambda}{1-\lambda} [N + O(1)] \|Z_a^u\|^2 \Pi_a^u(d\lambda).$$

The expectation on the right-hand side of limit 2.2 can be written as

$$\frac{1}{a^2 t} \sum_{N=1}^{\infty} \mathbb{E}_v \left[\left(\sum_{j=0}^{N-1} Z_{a,j}^u \right)^2 \right] \mathbb{P}(N_{a,t} = N) = \int_{-1}^1 \frac{1+\lambda}{1-\lambda} \mathbb{E}_v \left[\frac{N_{a,t} + O(1)}{ah(a)t} \right] \frac{h(a)}{a} \|Z_a^u\|^2 \Pi_a^u(d\lambda).$$

Keeping in mind the relationship between the expectation of $N_{a,t}$ and $\mathbb{E}_v[\tau_b]$ observed above in the derivation of the i.i.d. case, we have

$$\lim_{a \rightarrow \infty} \frac{1}{a^2 t} \mathbb{E}_v \left[\left(\sum_{j=0}^{N_{a,t}-1} Z_{a,j}^u \right)^2 \right] = \lim_{a \rightarrow \infty} \frac{h(a)}{a} \frac{\mathbb{E}_v \left[(Z_a^u)^2 \right]}{\mathbb{E}_v[\tau_b]} \int_{-1}^1 \frac{1+\lambda}{1-\lambda} \Pi_a^u(d\lambda) = \mathcal{D}_0 \int_{-1}^1 \frac{1+\lambda}{1-\lambda} \Pi^u(d\lambda).$$

This proves the claimed form of the diffusion constant. The necessary central limit theorem and weak invariance principle required to prove convergence to Brownian motion (in the case $n - k = 1$) will be shown later. \square

We remark now on a simple interpretation of the diffusivity \mathcal{D} in the context of the idealized experiment described earlier that allows us to obtain \mathcal{D} without recourse to the somewhat physically artificial a -scaling. In order to keep the discussion simple, only the case $k = 1$ is considered, although the main idea can be generalized in obvious ways.

Consider a channel $\mathcal{C}(L) = [-L, L] \times \mathbb{B}^{n-1}(r)$ of length $2L$ and recall that $\tau(L, r, s)$ is the mean exit time from $\mathcal{C}(L)$, introduced in Subsection 1.1, where s is root-mean-square speed. The following elementary dimensional properties are easily derived:

- (i) $\tau(L, r, s) = \tau(aL, ar, as)$
- (ii) $\tau(L, r, s) = a\tau(L, r, as)$
- (iii) $\tau(aL, r, s) = ah(a)\tau(L, r/a, h(a)s)$

where the third property is a consequence of the first two. It also follows from (i) and (ii) that the function $F(L/r) := (s/r)\tau(L, r, s)$ is independent of s , dimensionless (that is, devoid of physical units), and scale invariant.

We are interested in the asymptotic behavior of $\tau(L, r, s)$ as L grows to infinity. Since the mean exit time from the interval $[-r, r]$ for Brownian motion with diffusivity \mathcal{D} starting at 0 is r^2/\mathcal{D} we expect, given Theorem 1 and the above properties of the mean exit time,

$$(2.3) \quad \tau(L, r, s) \sim \begin{cases} \frac{L^2}{\mathcal{D}} & \text{if } n - k \geq 2 \\ \frac{L^2}{\mathcal{D} \ln(L/r)} & \text{if } n - k = 1. \end{cases}$$

Notice, in particular, the expected relation

$$\mathcal{D} = C(P)rs,$$

where $C(P) = \lim_{a \rightarrow \infty} ah(a)/F(a)$, being independent of L, r, s , is a characteristic number of the scattering process at a microscopic scale. This asymptotic expression is indeed true, and it is a consequence of the following proposition, which will be proved later.

Proposition 3. *Let $L > 0$ and \mathcal{T} be the function on the space of continuous paths $\gamma : [0, \infty) \rightarrow \mathbb{R}$ defined by $\mathcal{T}(\gamma) := \inf\{t \geq 0 : |\gamma(t)| \geq L\}$, where the infimum of the empty set is taken to be $-\infty$. Let \mathbb{E}_0^a denote expectation with respect to the law of the process $t \mapsto X_{a,t}$, conditioned to start at 0 and \mathbb{E}_0^B , similarly defined, for the Brownian motion with diffusion constant \mathcal{D} . Then*

$$\lim_{a \rightarrow \infty} \mathbb{E}_0^a[\mathcal{T}] = \mathbb{E}_0^B[\mathcal{T}] = \mathcal{D}^{-1}L^2$$

and the asymptotic expression 2.3 holds.

2.3 GENERALIZED MAXWELL-SMOLUCHOWSKI MODELS

Before examining diffusivity in examples of collision operators derived from geometric microstructures, we briefly mention an interesting generalization of a very classical example widely used in kinetic theory of gases, known as the *Maxwell-Smoluchowski* collision model. The collision operator for this model is $P_{\text{MS}} = \alpha Q_\beta + (1 - \alpha)I$, where $\alpha \in [0, 1]$ is a constant, I is the identity operator, and Q_β is the projection into the subspace of constant functions:

$$(Q_\beta \varphi)(v) := \int_{\mathbb{H}} \varphi(u) d\mu_\beta(u).$$

The interpretation is that, upon collision with the surface, a particle scatters according to μ_β (diffuse scattering; see definition of μ_β at the beginning of Subsection 1.2) with probability α , and reflects specularly with probability $1 - \alpha$. Clearly, P_{MS} is a natural collision operator according to Definition 1. A similar definition can be made for random reflection operators,

with μ in place of μ_β . In either case, the diffusivity is easily shown to be $\mathcal{D} = \frac{1+p}{1-p} \mathcal{D}_0$, where $p = 1 - \alpha$ is the probability of specular reflection and $\{1, p\}$ is the spectrum of P_{MS} . This simple model is very useful in providing a rough interpretation of the typical η obtained from microstructures.

A generalization is as follows. Let Q be a collision operator, not necessarily natural, such that for $v \in \mathbb{H}$ the measure

$$A \mapsto Q(v, A) := (Q \mathbb{1}_A)(v)$$

is absolutely continuous with respect to the standard area measure, where A is a measurable set and $\mathbb{1}_A$ denotes its indicator function. We say that operators such as Q are *diffuse*. Let $\alpha : \mathbb{H} \times \mathbb{H} \rightarrow [0, 1]$ be a measurable function. Now form the *Metropolis-Hastings kernel* with proposal Q and acceptance probability α . The corresponding operator is

$$(P\varphi)(v) = \varphi(v) + \int_{\mathbb{H}} \alpha(v, u) [\varphi(u) - \varphi(v)] Q(v, du).$$

The interpretation is that, for an incoming velocity v , a candidate outgoing velocity V is chosen according to $Q(v, \cdot)$; then, with probability $\alpha(v, V)$, V is accepted as the post-collision velocity, and with probability $1 - \alpha(v, V)$ the post-collision velocity is taken to be v itself.

The standard Metropolis-Hastings method provides an explicit α for a given Q such that the resulting P is natural with respect to μ_β . See [26] for the general construction. This provides a large class of examples of natural collision operators satisfying the following definition.

Definition 2 (Generalized Maxwell-Smoluchowski models). *We say that the collision operator P defines a generalized Maxwell-Smoluchowski model if it is a natural operator for a given μ_β and is of the Metropolis-Hastings type with a diffuse proposal operator Q and acceptance function α .*

Two families of examples of generalized Maxwell-Smoluchowski models are given in the next section. In the family where a flat transition of (scale-free) length h is added between semicircles, the proposal Q is simply the operator associated to the semicircle geometry and the acceptance function is the constant $1 - h$. In the family where the semicircle is split and a flat floor of length h is added, the acceptance function is more complicated as it depends on the incoming pre-collision angle.

Regarding these operators and their diffusivities, we only indicate the following very general comparison result. Let P_1 and P_2 be natural collision operators with the same stationary distribution μ . We say that P_1 *dominates* P_2 *off the diagonal* if $P_1(v, A \setminus \{v\}) \geq P_2(v, A \setminus \{v\})$ for μ -almost all v . The next proposition holds with little modification to what is given in [26].

Proposition 4. *Let P_1 and P_2 be natural collision operators and let \mathcal{D}_1 and \mathcal{D}_2 be the associated diffusivities for the limit Brownian motion process in the scaled channel system. If P_1 dominates P_2 off the diagonal then $\mathcal{D}_1 \leq \mathcal{D}_2$.*

In other words, an operator that is more dispersing in the sense just defined has slower diffusion. This result is illustrated by the example of Figure 2.3 of the next section featuring a flat transition between semicircles. The formula for $\mathcal{D}(h)$ (next section) shows that the diffusivity increases with h , which is what is expected from the proposition. A similar comparison of operators does not hold for the example shown below where a flat floor is added.

2.4 EXAMPLES OF DIFFUSIVITY FOR GEOMETRIC MICROSTRUCTURES

We limit our attention in this subsection to operators associated to static microstructures in dimension 2. Therefore, the main question of interest is how the shape of the surface contour influences the signature parameter $\eta = \mathcal{D}/\mathcal{D}_0$ of the particle-surface interaction. For the examples given here, η can be obtained exactly. It will be noticed that the examples are variations on a theme: they are built out of arcs of circle and straight lines and correspond to focusing billiards.



Figure 2.2: A geometric microstructure consisting of semicircular arcs.

For the focusing semicircle structure of Figure 2.2 it will be shown that

$$(2.4) \quad \eta = \frac{1 - \frac{1}{4} \log 3}{1 + \frac{1}{4} \log 3}.$$

This value is reminiscent of the limit variance seen in central limit theorems for the stadium billiard of deterministic billiard dynamics (see [4]).

A simple modification of the semicircles contour is shown in Figure 2.3. It consists of semicircles as in the first example separated by flat sections. We introduce the parameter $h = l/(l + 2r) \in (0, 1)$, which gives the proportion of the top line occupied by the flat part.



Figure 2.3: Circles and flats. For the non-periodic shape on the right, we assume that the fraction of length comprising the flat part on top is well defined and equal to $h = l/(l + 2r)$, where l and r are described on the left figure. The parameter η is the same in both cases.

The diffusivity for the shapes of Figure 2.3, as a function of h , is given by

$$(2.5) \quad \mathcal{D}(h) = \mathcal{D}_0 \frac{\eta + h}{1 - h}$$

where η is the signature diffusivity parameter of the example of Figure 2.2. Clearly, for the $h = 0$ limiting case, the microscopic cell is simply the semicircle and $\mathcal{D}(0) = \mathcal{D}$. At the other end, as h approaches 1 the diffusivity increases without bound. Of course, for a completely flat surface, the transport ceases to be a diffusion at all and becomes (a much faster) deterministic motion.

The next example refers to the surface of Figure 2.4. In this case, the parameter h measures the length of the middle wall relative to the period length of the contour.



Figure 2.4: Semicircles with middle wall. Define the scale free parameter $h = l/(2r)$.

For the middle wall of relative height $h < 1/2$ and $h = 1/2$, the values are, respectively,

$$(2.6) \quad \mathcal{D}(h) = \mathcal{D}_0 \frac{1 - \frac{1}{4} \log 3}{1 + \frac{1}{4} \log 3}, \quad \mathcal{D}(1/2) = \mathcal{D}_0 \frac{1 + \frac{1}{4} \log 3}{1 - \frac{1}{4} \log 3}.$$

Observe, in particular, that the diffusivity does not change, and has the same η as the example of Figure 2.2, until the middle walls reach the top of the cell. At that point the diffusivity changes discontinuously to $\mathcal{D}(1/2)$.

A related phenomenon is seen in the next family of examples, shown in Figure 2.5. It is obtained from the first example by adding a flat floor of relative length $h = l/(l + 2r) \in [0, 1)$. It will be shown for this parametric family that

$$(2.7) \quad \mathcal{D}(h) = \mathcal{D}_0 \frac{1 + \zeta_h}{1 - \zeta_h},$$

where

$$\zeta_h = -\frac{1 + 3h}{4} \frac{1 - h}{1 + h} \log \frac{3 + h}{1 - h}.$$



Figure 2.5: A family of geometric microstructures with parameter $h = l/(l + 2r)$.

At the $h = 0$ limit we naturally have the same η as for the first example. What happens when h approaches 1 is perhaps more surprising. In this case $\mathcal{D}(h)$ approaches the baseline value \mathcal{D}_0 . Recall that this is the diffusivity of the process where at each collision event the particle reflects, independent of the pre-collision angle, according to the stationary measure μ . From the perspective of a single collision event, collisions are nearly mirror-like; on the other hand, from a multiple scattering perspective the collision process reaches equilibrium instantaneously making the surface ideally rough in a sense. This peculiar phenomenon and the discontinuity in \mathcal{D} seen in the previous example are due to the fact that the diffusivity is determined only by collisions which occur at angles nearly parallel to the channel walls, a result made explicit in Proposition 7. An allusion to this property is found in [6].

The computation of \mathcal{D} for these examples will be given in Section 4.

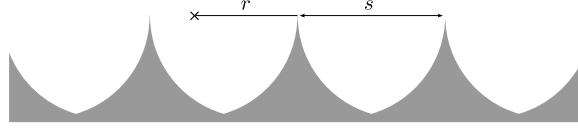


Figure 2.6: The family of geometric microstructures of Figure 2.5 includes the above when l is allowed to be negative. Let $l = s - 2r$, where r is the radius of the arcs of circle and s is the width of a period cell and s is the length of the opening. For $l \geq -r$, the diffusivity $\mathcal{D}(h)$, parametrized by $h = l/(l + 2r)$, is still given by Equation 2.7.

3 THE MAIN LIMIT THEOREMS IN THE INFINITE VARIANCE CASE

Let P be a natural collision operator with stationary measure ν . Define for each $\nu \in \mathbb{H}$ the measure $P(\nu, A) = (P\mathbb{1}_A)(\nu)$ for $A \subset \mathbb{H}$ measurable. Let $\Omega = \mathbb{H}^{\mathbb{N}}$ and denote by \mathcal{F} the product Borel σ -algebra. Define a measure \mathbb{P} on cylinder sets as

$$\mathbb{P}(\{\omega \in \Omega : \omega_0 \in A_0, \dots, \omega_n \in A_n\}) = \int_{A_0} \int_{A_1} \dots \int_{A_n} P(\omega_{n-1}, d\omega_n) \dots P(\omega_0, d\omega_1) \mu(d\omega_0),$$

for $A_0, \dots, A_n \subset \mathbb{H}$ measurable and extend it to \mathcal{F} . The coordinate projections $V_i : \Omega \rightarrow \mathbb{H}$ given by $V_i(\omega) = \omega_i$, for $i = 0, 1, \dots$, thought of as random variables on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$, constitute a Markov chain. Because ν is stationary for P , it follows that the Markov chain is stationary.

Being a natural operator, P together with ν satisfy the detailed balance condition, which implies it is self-adjoint on $L^2(\mathbb{H}, \nu)$. We also assume from now on that P is quasi-compact, and so has a *spectral gap*. These assumptions imply that the chain is ρ -mixing. That is,

$$\sup \left\{ \text{corr}(X, Y) : X \in L^2(\mathcal{F}_0^k), Y \in L^2(\mathcal{F}_{k+n}^\infty), k \geq 1 \right\} = O(\rho^n),$$

for some ρ such that $0 < \rho < 1$, where the notations are as follows: $\text{corr}(X, Y)$ is the correlation between X and Y , $L^2(\mathcal{F}_0^k)$ is the space of square integrable functions measurable with respect to the σ -algebra \mathcal{F}_0^k generated by V_0, \dots, V_k and $L^2(\mathcal{F}_{k+n}^\infty)$ is the space of square integrable functions for the σ -algebra generated by V_j , for $j \geq k + n$.

Consider the a -scaled channel system, as defined earlier, with channel radius scaled down by a and each post-collision velocity scaled up by the previously defined $h(a)$. Let $X_{a,t}$ be the position at time t along the horizontal axis of the particle for the a -scaled random flight starting at $X_{a,0} = 0$; let $N_{a,t}$ be the number of collisions with the walls for the scaled system during the time interval $[0, t]$. Notice that $N_{a,t} = N_{ah(a)t}$, where N_s is, by definition, the number of collisions during $[0, s]$ for the non-scaled system.

In what follows, $h(a) = a/\log a$ and Z will be any real measurable function on \mathbb{H} *slowly varying* at infinity, in the sense that $\mathbb{E}_\nu[Z^2 \mathbb{1}_{|Z| \leq a}] \sim C \log a$ as $a \rightarrow \infty$, where $C > 0$ is a constant and

a_n/b_n means $a_n/b_n \rightarrow 1$ as $n \rightarrow \infty$. The various notations used before for the inter-collision displacement function will be used for this general Z . Thus, for example, $Z_j = Z(V_j)$. However, the a -truncation Z_a of Z will be understood more generally as follows: If $I(a)$ is an interval whose endpoints are functions of the scaling parameter, we write $Z^{I(a)} := Z \mathbb{1}_{\{Z \in I(a)\}}$, and if there is no ambiguity about which interval is being assumed we write $Z_a := Z^{I(a)}$. Combining notations, $Z_{a,j} = Z_a(V_j)$, for the non-scaled observable Z , while the corresponding a -scaled quantity (for the a -scaled system with radius r/a and root-mean-square speed $h(a)s$) is $a^{-1}Z_{a,j}$. Unless explicitly stated otherwise, Z_a is associated to the interval $I(a) = [-a, a]$. The probability measure $\Pi_a(d\lambda)$ on the spectrum on P is defined as before for a general Z : $\Pi_a(d\lambda) := \|Z_a\|^{-2} \langle Z_a, \Pi(d\lambda) Z_a \rangle$. While we make no claims on the existence of a weak limit of the measures Π_a we note that there exists a subsequence of Π_a that converges weakly to a probability measure which we will call Π_0 .

If a sequence of random variables converges in distribution to a normal random variable with mean 0 and variance σ^2 , we say for short that the sequence converges to $\mathcal{N}(0, \sigma^2)$.

Theorem 2 (Central limit theorem). *Suppose P is a quasi-compact natural operator and that Assumption 1 holds. Then, for any $t > 0$, the sum $\sum_{j=0}^{N_{a,t}-1} a^{-1} Z_j$ converges to $\mathcal{N}(0, t\mathcal{D})$ as $a \rightarrow \infty$, where*

$$\mathcal{D} = \lim_{a \rightarrow \infty} \frac{1}{a^2 t} \mathbb{E}_v \left[\left(\sum_{j=0}^{N_{a,t}-1} Z_{a,j} \right)^2 \right].$$

Theorem 3 (Weak invariance principle). *Under the same assumptions as in Theorem 1, let $X_{a,t} \in \mathbb{R}^k$ be the particle at time t in the a -scaled system with radius r/a and root-mean-square velocity $h(a)s$. Then $X_{a,t}$ converges weakly to B_t , a Brownian motion with diffusivity given by the quadratic form \mathcal{D}^u .*

We note that it is still possible, without Assumption 1, to prove a central limit theorem and weak invariance principle for the inter-collision displacements—only slight modifications of the statements and proofs are needed. However, Assumption 1 allows us to express the variance of the limit distribution in the central limit theorem in terms of the observable Z and the operator P . So while more general statements can be made and proven, we choose when possible to emphasize the connection between macroscopic data—the limit variance in the central limit theorem—and microscopic data encoded in the operator P and its spectrum.

We also note that Assumption 1 may be reduced to a statement about covariances. Observe that

$$\mathbb{E} \left[\left(\sum_{j=0}^{N_{a,t}-1} a^{-1} Z_{a,j} \right)^2 \right] = \mathbb{E} \left[a^{-2} \sum_{j=0}^{N_{a,t}-1} Z_{a,j}^2 \right] + \mathbb{E} \left[a^{-2} \sum_{0 < |i-j| < N_{a,t}} Z_{a,i} Z_{a,j} \right].$$

As already seen in the proof of Theorem 1 the limit of the first summand exists in general. Thus the assumption may be restated as requiring the existence of the limit of the second summand of covariances. In the case of strictly stationary ρ -mixing sequences with finite variance and a relatively light (less than exponential) condition on the rate of mixing, the scaled limit of variances is known to always exist (see for example [7]). As far as we are aware, the corresponding result in our setting—whether such a limit always exists for exponentially fast ρ -mixing stationary sequences with infinite variance—has not been addressed.

The remainder of the paper is organized as follows. Section 3.1 outlines the proof of the central limit theorem as a sequence of technical lemmas, leaving the proofs of the lemmas for Section 5.2. In Section 3.2 we prove the weak invariance principle and Proposition 3 on convergence of mean exit times. The computation of diffusivity for the examples of Section 2.4 is given in Section 4. The first subsection there outlines a general technique for such computations, while the last two subsections are devoted to the computation of diffusivity for a periodic focusing semicircle micro-geometry and related parametric families.

3.1 OUTLINE OF PROOF OF THE CENTRAL LIMIT THEOREM

In this section we explain the skeleton of the proof of Theorem 2 as a sequence of lemmas, leaving the proofs of the lemmas for Section 5.2. Now Z represents more generally an integrable scalar (rather than vector) random variable so that $\mathbb{E}[|Z|] < \infty$, having mean 0 and slowly varying at infinity; that is, $\mathbb{E}[(Z_a)^2] = O(\ln a)$. Although Z is more general than before, we find it convenient to continue to refer to Z as the *displacement*. The typical random variable we wish to apply the below theorems to are the projections of the displacement vector Z^u considered before. For a channel in \mathbb{R}^2 bounded by parallel lines, we are mainly interested in $Z(v) = r v_1 / v_2$, where $v = (v_1, v_2)$, with vector $(0, 1)$ being perpendicular to the boundary lines.

Lemma 1. *Let τ_b be the random inter-collision time. Then $(ah(a)t)^{-1} N_{a,t}$ converges to $1/\mathbb{E}_v[\tau_b]$ almost surely for each $t > 0$ as $a \rightarrow \infty$. In particular, let*

$$n_{a,t} := \left\lfloor \frac{ah(a)t}{\mathbb{E}_v[\tau_b]} \right\rfloor,$$

where $[x]$ denotes the integer part of x . Then $N_{a,t}/n_{a,t} \rightarrow 1$ almost surely.

The proof of Lemma 1 has already been given in the proof of Theorem 1 in Section 2.2.

Lemma 2. *Let $n_{a,t}$ be defined as in Lemma 1. If $\sum_{j=0}^{n_{a,t}-1} a^{-1} Z_j$ converges in distribution to $\mathcal{N}(0, t\mathcal{D})$ then so does $\sum_{j=0}^{N_{a,t}-1} a^{-1} Z_j$.*

The next lemma shows that one can work with the a -truncated random variables $Z_{a,j}$ instead of the Z_j .

Lemma 3. *The quantity $\sum_{j=0}^{n_{a,t}-1} a^{-1} (Z_j - Z_{a,j})$ converges to 0 in probability as $a \rightarrow \infty$.*

To address the issue of statistical dependence among the displacements, we employ Bernstein's big-small block technique. That is, we break the sum of truncated displacements into alternating big and small blocks in such a way that the small blocks are negligible and the big blocks are in a sense independent. Let $\alpha = 0.01, \beta = 0.6$ and define $b_{a,t} = \lfloor n_{a,t}^\beta \rfloor$ and $s_{a,t} = \lfloor n_{a,t}^\alpha \rfloor$. These are the lengths of the big blocks and small blocks, respectively. Define the big blocks as

$$U_{a,i} = \sum_{j=1}^{b_{a,t}} a^{-1} Z_{a,(i-1)(b_{a,t}+s_{a,t})+j},$$

for $1 \leq i \leq k_{a,t}$, where $k_{a,t}$ is the largest integer i for which $(i-1)(b_{a,t} + s_{a,t}) + b_{a,t} < n_{a,t} - 1$. Note that $k_{a,t} \sim n_{a,t}^{1-\beta}$. Next define the small blocks $V_{a,i}$ as the sums that remain between the big blocks. That is,

$$V_{a,i} = \sum_{j=1}^{s_{a,t}} a^{-1} Z_{a,(i-1)(b_{a,t} + s_{a,t}) + b_{a,t} + j},$$

for $1 \leq i < k_{a,t}$, and $V_{a,k_{a,t}} = a^{-1} (Z_{a,(k_{a,t}-1)(b_{a,t} + s_{a,t}) + b_{a,t} + 1} + \cdots + Z_{a,n_{a,t}-1})$, so that

$$\sum_{j=0}^{n_{a,t}-1} a^{-1} Z_{a,j} = \sum_{i=1}^{k_{a,t}} (U_{a,i} + V_{a,i}).$$

The next lemma shows that it will suffice to consider only the big blocks as the sum of the small blocks is negligible in probability.

Lemma 4. *The sum $\sum_{i=1}^{k_{a,t}} V_{a,i}$ converges to 0 in probability as $a \rightarrow \infty$.*

The proof of Theorem 2 has by now been reduced to showing that $\sum_{i=1}^{k_{a,t}} U_{a,i} \rightarrow \mathcal{N}(0, t\mathcal{D})$ as $a \rightarrow \infty$. Therefore, the theorem will be proved if we show that the characteristic function of this sum converges to the characteristic function of the normal random variable. By the next lemma, the big blocks are asymptotically independent in the sense that the characteristic function of their sum can be estimated by the product of their characteristic functions.

Lemma 5. *Convergence $\left| \mathbb{E} \left[\exp \left(i\mu \sum_{i=1}^{k_{a,t}} U_{a,i} \right) \right] - \prod_{i=1}^{k_{a,t}} \mathbb{E} \left[\exp (i\mu U_{a,i}) \right] \right| \rightarrow 0$ holds for all μ in \mathbb{R} as $a \rightarrow \infty$.*

Combining the above with the following lemma then gives the proof of Theorem 2.

Lemma 6. *The convergence $\prod_{i=1}^{k_{a,t}} \mathbb{E} \left[\exp (is U_{a,i}) \right] \rightarrow \exp \left(-\frac{s^2}{2} t\mathcal{D} \right)$ holds for all $s \in \mathbb{R}$ as $a \rightarrow \infty$.*

3.2 PROOF OF THE WEAK INVARIANCE PRINCIPLE

We give now a proof of Theorem 3 and of Proposition 3. To show weak convergence in the space $C[0, \infty) := C([0, \infty), \mathbb{R}^k)$ of continuous paths in \mathbb{R}^k it suffices to show that the finite dimensional distributions of the projection of X_a along each coordinate axis of \mathbb{R}^k converge weakly to those of Brownian motion B and the collection X_a in $C[0, \infty)$ is tight (see, for example, [5]). In fact, with regard to the second condition it suffices to show tightness of the collection restricted to $C[0, t]$ for all $t > 0$ (see, for example, [28]). Thus the following two propositions are sufficient to prove the theorem. We assume without loss of generality that dimension $k = 1$.

Proposition 5. *Under the conditions of Theorem 3, the random vectors $(X_{a,t_1}, \dots, X_{a,t_l})$ converge weakly to $(B_{t_1}, \dots, B_{t_l})$ as $a \rightarrow \infty$ for all l and all $t_1 < \cdots < t_l \in [0, \infty)$.*

Proof. The proof is by induction on k . For the case $k = 1$ we begin by writing

$$X_{a,t_1} = \left(\sum_{j=0}^{N_{a,t_1}-1} a^{-1} Z_j \right) + R_{a,t_1},$$

where R_{a,t_1} is the signed distance traveled in the time between collision N_{a,t_1} and t_1 . We claim that $R_{a,t_1} \rightarrow 0$ in probability as $a \rightarrow \infty$. Indeed note that $|R_{a,t_1}| \leq |a^{-1} Z_{N_{a,t_1}}|$ so, for any $\epsilon > 0$

$$\mathbb{P}(|R_{a,t_1}| > \epsilon) \leq \mathbb{P}\left(|a^{-1} Z_{N_{a,t_1}}| > \epsilon\right) \leq \frac{\mathbb{E}[|Z|]}{\epsilon a},$$

which goes to 0 as $a \rightarrow \infty$. It follows that X_{a,t_1} converges in distribution to B_{t_1} by Theorem 2.

Next we consider the case $l > 1$. It suffices to show that $\sum_{i=1}^l \xi_i X_{a,t_i}$ converges in distribution to $\sum_{i=1}^l \xi_i B_{t_i}$ as $a \rightarrow \infty$ for any $(\xi_1, \dots, \xi_l) \in \mathbb{R}^l$. We first write

$$\sum_{i=1}^l \xi_i X_{a,t_i} = \xi_1 X_{a,t_1} + \dots + \xi_{l-2} X_{a,t_{l-2}} + (\xi_{l-1} + \xi_l) X_{a,t_{l-1}} + \xi_l (X_{a,t_l} - X_{a,t_{l-1}})$$

Arguing as in the previous case and using the techniques of truncation and Bernstein's method as in the proof of the central limit theorem we conclude that the first $l-1$ summands above are asymptotically independent from the last so that, by the induction hypothesis, the sum

$$\xi_1 X_{a,t_1} + \dots + \xi_{l-2} X_{a,t_{l-2}} + (\xi_{l-1} + \xi_l) X_{a,t_{l-1}} + \xi_l (X_{a,t_l} - X_{a,t_{l-1}})$$

converges in distribution as $a \rightarrow \infty$ to

$$\xi_1 B_{t_1} + \dots + \xi_{l-2} B_{t_{l-2}} + (\xi_{l-1} + \xi_l) B_{t_{l-1}} + \xi_l B_{t_l - t_{l-1}} = \sum_{i=1}^l \xi_i B_{t_i}.$$

This concludes the proof of the proposition. \square

Proposition 6. Let $t > 0$ and define $u(a, \delta) := \sup \{|X_{a,u} - X_{a,v}| : |u - v| < \delta \text{ and } u, v \in [0, t]\}$. Then $\lim_{\delta \rightarrow 0} \lim_{a \rightarrow \infty} \mathbb{P}(u(a, \delta) > \epsilon) = 0$ for all $\epsilon > 0$.

Proof. Let $\epsilon > 0$ and $\delta < t$. For simplicity we assume δ divides t and let $n = t/\delta$. The argument holds in general with only minor modification. Let $0 = t_0 < \dots < t_n = t$ be the equidistant partition of $[0, t]$. Observe that

$$\mathbb{P}(u(a, \delta) > \epsilon) \leq \mathbb{P}\left(\max_{0 \leq j \leq n-1} \sup_{s \in [t_j, t_{j+1}]} |X_{a,s} - X_{a,t_j}| > \epsilon/3\right) \leq \sum_{j=0}^{n-1} \mathbb{P}\left(\sup_{s \in [t_j, t_{j+1}]} |X_{a,s} - X_{a,t_j}| > \epsilon/3\right).$$

Introducing the notation $D_k^l := \sum_{j=k}^{l-1} Z_{a,j} - \sum_{j=k}^{N_{a,t}-1} Z_{a,t}$, then for any $0 \leq j \leq n-1$, the event $\sup \{|X_{a,s} - X_{a,t_j}| : s \in [t_j, t_{j+1}]\} > \epsilon/3$ implies that $\max_{N_{a,t_j} \leq k \leq N_{a,t_{j+1}}+1} |D_0^k| > a\epsilon/6$. Next let $n_\delta = \left\lfloor \frac{ah(a)\delta}{v/r\pi} \right\rfloor$ and let $A(j, \delta)$ denote the event $N_{a,t_{j+1}} - N_{a,t_j} + 1 \leq n_\delta$. Then the probability $\mathbb{P}\left(\sup_{s \in [t_j, t_{j+1}]} |X_{a,s} - X_{a,t_j}| > \epsilon/3, A(j, \delta)\right)$ is bounded above by

$$\begin{aligned} \mathbb{P}\left(\max_{N_{a,t_j} \leq k \leq N_{a,t_{j+1}}+1} |D_0^k| > a\epsilon/6, A(j, \delta)\right) &\leq \mathbb{P}\left(\max_{N_{a,t_j} \leq k \leq N_{a,t_j}+n_\delta} |D_0^k| > a\epsilon/6\right) \\ &\leq 2\mathbb{P}\left(\max_{1 \leq k \leq n_\delta} \left|\sum_{i=0}^{k-1} Z_i\right| > a\epsilon/6\right) \leq 4\mathbb{P}\left(\left|\sum_{i=0}^{n_\delta-1} Z_i\right| > a\epsilon/6\right), \end{aligned}$$

where the last two inequalities follow as in the proof of Lemma 2. Therefore,

$$\begin{aligned} \mathbb{P}(u(a, \delta) > \epsilon) &\leq \sum_{j=0}^{n-1} \mathbb{P} \left(\sup_{s \in [t_j, t_{j+1}]} |X_{a,s} - X_{a,t_j}| > \epsilon/3 \right) \leq \sum_{j=0}^{n-1} \left(4\mathbb{P} \left(\left| \sum_{i=0}^{n_\delta-1} Z_i \right| > a\epsilon/6 \right) + \mathbb{P}(A(j, \delta)^c) \right) \\ &= n \left(4\mathbb{P} \left(\left| \sum_{i=0}^{n_\delta-1} Z_i \right| > a\epsilon/6 \right) + \mathbb{P}(A(j, \delta)^c) \right) = \frac{t}{\delta} \left(4\mathbb{P} \left(\left| \sum_{i=0}^{n_\delta-1} Z_i \right| > a\epsilon/6 \right) + \mathbb{P}(A(j, \delta)^c) \right). \end{aligned}$$

Notice that the number of collisions in the interval $[t_j, t_{j+1}]$ is precisely $N_{a,t_{j+1}} - N_{a,t_j} + 1$ and so by Lemma 1, $\frac{1}{n_\delta} (N_{a,t_{j+1}} - N_{a,t_j} + 1) \rightarrow 1$ almost surely as $a \rightarrow \infty$. From this it follows that $\mathbb{P}(A(j, \delta)^c) \rightarrow 0$ almost surely as $a \rightarrow \infty$, independent of j and δ . From Theorem 2

$$\frac{1}{\delta} \mathbb{P} \left(\left| \sum_{i=0}^{n_\delta-1} a^{-1} Z_i \right| > \epsilon/6 \right) \rightarrow \frac{2}{\delta^{3/2} \sqrt{2\pi\mathcal{D}}} \int_{\epsilon/6}^{\infty} e^{-x^2/2\delta\mathcal{D}} dx$$

as $a \rightarrow \infty$. Letting $\delta \rightarrow 0$ on the right-hand side above then gives the result. \square

Proof of Proposition 3. The equality in the statement of the proposition is a standard fact on the mean exit time of Brownian motion from an interval. We prove here only the convergence of mean exit times. Note that by the continuous mapping theorem $\tau(X_a)$ converges in distribution to $\tau(B)$. (Of course τ is not continuous on all of $C[0, \infty)$ but it's not difficult to show that it is \mathbb{P}_0^B -a.s. continuous.) Therefore, to show the convergence of mean exit times it suffices to show that the collection of $\tau(X_a)$ is uniformly integrable. That is, it suffices to show that for any $\epsilon > 0$ there exists $M > 0$ such that $\mathbb{E}_0^a [\tau \mathbb{1}_{\{\tau > M\}}] < \epsilon$ for all a .

Note that for all $\epsilon > 0$ there exists $\delta \in (0, 1)$ such that $\mathbb{P}_x^B(\tau < \epsilon) > \delta$ for all $x \in (-L, L)$. Since $\tau(X_a)$ converges to $\tau(B)$ in distribution it follows, similarly, that for any $\epsilon > 0$ there exists some $\delta \in (0, 1)$ and a_0 such that $\mathbb{P}_x^a(\tau < \epsilon) > \delta$ for all $a \geq a_0$ and for all $x \in (-L, L)$. If we let $\epsilon = 1$ and let δ be the corresponding value in $(0, 1)$ then it follows by induction and the strong Markov property that $\mathbb{P}_0^a(\tau > k) \leq (1 - \delta)^k$ for every positive integer k and $a \geq a_0$. Therefore, if we choose M' large enough so that $\sum_{k=M'}^{\infty} (k+1)(1 - \delta)^k < \epsilon$, then for $a \geq a_0$

$$\mathbb{E}_0^a [\tau \mathbb{1}_{\{\tau > M'\}}] \leq \sum_{k=M'}^{\infty} (k+1) \mathbb{P}_0^a(\tau > k) \leq \sum_{k=M'}^{\infty} (k+1)(1 - \delta)^k < \epsilon.$$

It is also straightforward to see that there exists $M'' > 0$ such that $\mathbb{E}_0^a [\tau \mathbb{1}_{\{\tau > M''\}}] < \epsilon$ for $a < a_0$. Letting $M = \max\{M', M''\}$ then gives the uniform integrability. \square

4 EXAMPLES

This section is devoted to showing how the diffusivity \mathcal{D} encodes surface microscopic structure when our operator P represents a *random reflection*. The structure of the section is as follows. The first subsection gives a general outline for computing \mathcal{D} independent of any given surface microscopic structure. The second subsection computes \mathcal{D} in the case that the surface of the walls is given by a periodic arrangement of focusing semicircles. The last subsection gives \mathcal{D} for certain parametric families of surfaces derived from the semicircle example of the previous subsection.

4.1 GENERAL TECHNIQUE

While in general, under Assumption 1, the diffusivity is given by

$$t\mathcal{D} = \lim_{a \rightarrow \infty} \mathbb{E} \left[\left(a^{-1} \sum_{j=0}^{N_{a,t}-1} Z_j^{I(a)} \right)^2 \right],$$

where $I(a)$ is the interval given in Theorem 2, it is possible to consider a significantly reduced truncation without altering the value of \mathcal{D} .

Let $\eta \in (0, 1)$ and define $J(a) := \{x : \exp(\log^\eta a) < |x| < a/\log^\eta a\}$. The following proposition shows that we may use the truncated displacements $Z^{J(a)}$ in computing \mathcal{D} so that in fact a vanishingly small cone of trajectories determine the diffusivity.

Proposition 7. *Under the assumptions of Theorem 2,*

$$t\mathcal{D} = \lim_{a \rightarrow \infty} \mathbb{E} \left[\left(a^{-1} \sum_{j=0}^{N_{a,t}-1} Z_j^{J(a)} \right)^2 \right].$$

Proof. As in the proof of Theorem 1, the second moment on the right above may be expressed as the spectral integral

$$\mathbb{E} \left[\left(a^{-1} \sum_{j=0}^{N_{a,t}-1} Z_j^{J(a)} \right)^2 \right] = \int_{-1}^1 \frac{1+\lambda}{1-\lambda} \frac{\mathbb{E}[N_{a,t} + O(1)]}{ah(a)} \left(\frac{h(a)}{a} \|Z^{J(a)}\|^2 \right) \Pi_{Z^{J(a)}}(d\lambda).$$

where $\Pi_{Z^{J(a)}}(d\lambda) = \|Z^{J(a)}\|^{-2} \langle Z^{J(a)}, \Pi(d\lambda) Z^{J(a)} \rangle$ is a probability measure on the spectrum of P . Now observe that if $W := Z^{I(a) \setminus J(a)}$, then

$$\begin{aligned} \langle Z^{J(a)}, \Pi(d\lambda) Z^{J(a)} \rangle &= \langle Z^{I(a)} - W, \Pi(d\lambda) (Z^{I(a)} - W) \rangle \\ &= \langle Z^{I(a)}, \Pi(d\lambda) Z^{I(a)} \rangle - 2 \langle W, \Pi(d\lambda) Z^{I(a)} \rangle + \langle W, \Pi(d\lambda) W \rangle \end{aligned}$$

and $\|W\|_2^2 = O(\ln^\eta a)$. Therefore,

$$\left| \|Z^{J(a)}\|_2^2 - \|Z^{I(a)}\|_2^2 \right| \leq 2\|W\|_2 \|Z^{I(a)}\|_2 + \|W\|_2^2 = O(\ln^{\eta'} a)$$

for some $\eta' \in (0, 1)$. Multiplying both sides of the inequality by $h(a)/a = 1/\ln a$ and taking the limit as $a \rightarrow \infty$ implies that $Z^{J(a)}$ and $Z^{I(a)}$ grow at the same rate, and that in the limit formula for \mathcal{D} we can use $Z^{J(a)}$ rather than $Z^{I(a)}$. \square

With the previous proposition in mind we use the shorthand notation $Z_a := Z^{J(a)}$ through the rest of the subsection without the risk of ambiguity.

If we expand

$$\mathbb{E} \left[\left(a^{-1} \sum_{j=0}^{N_{a,t}-1} Z_{a,j} \right)^2 \right] = \mathbb{E} \left[a^{-2} \sum_{j=0}^{N_{a,t}-1} Z_{a,j}^2 \right] + \mathbb{E} \left[2a^{-2} \sum_{1 \leq i < j \leq N_{a,t}-1} Z_{a,i} Z_{a,j} \right],$$

the limit of the first term has been shown in the proof of Theorem 1 to be \mathcal{D}_0 , which is independent of the microstructure. Let $C(a)$ be a function that increases slower than $ah(a)$ but is

otherwise to be determined by a specific microstructure. For the second term we break the sum into two pieces as follows

$$a^{-2} \mathbb{E} \left[2 \sum_{1 \leq i < j \leq N_{a,t}-1} Z_{a,i} Z_{a,j} \right] = a^{-2} \mathbb{E} \left[\sum_{0 < |i-j| < C(a)} Z_{a,i} Z_{a,j} \right] + a^{-2} \mathbb{E} \left[\sum_{C(a) \leq |i-j| \leq N_{a,t}-1} Z_{a,i} Z_{a,j} \right].$$

The first term on the right above will be determined by the microstructure, but the second term actually vanishes.

Lemma 7. *We have $\lim_{a \rightarrow \infty} a^{-2} \mathbb{E} \left[\sum_{C(a) \leq |i-j| \leq N_{a,t}-1} Z_{a,i} Z_{a,j} \right] = 0$.*

Proof. Observe that

$$\begin{aligned} a^{-2} \sum_{C(a) \leq |i-j| \leq N_{a,t}-1} |\mathbb{E} [Z_{a,i} Z_{a,j}]| &= a^{-2} \sum_{i=1}^{N_{a,t}-C(a)} \sum_{j=i}^{N_{a,t}-C(a)} |\mathbb{E} [Z_{a,i} Z_{a,j+C(a)}]| \\ &= 2a^{-2} \mathbb{E} [Z_{a,0}^2] \sum_{i=1}^{N_{a,t}-C(a)} \sum_{j=i}^{N_{a,t}-C(a)} |\text{corr}(Z_{a,i}, Z_{a,j+C(a)})| \\ &\leq 2a^{-2} \mathbb{E} [Z_{a,0}^2] \sum_{i=1}^{N_{a,t}-C(a)} \sum_{j=i}^{N_{a,t}-C(a)} |\rho(C(a) + j - i)| \\ &\leq \frac{M}{ah(a)} \sum_{i=1}^{N_{a,t}-C(a)} \sum_{j=i}^{N_{a,t}-C(a)} \rho^{C(a)+j-i}, \end{aligned}$$

where $M > 0$ is a constant and $0 < \rho < 1$ is the essential spectral radius. Further,

$$\sum_{i=1}^{N_{a,t}-C(a)} \sum_{j=i}^{N_{a,t}-C(a)} \rho^{C(a)+j-i} = \frac{\rho^{C(a)}}{1-\rho} \left(N_{a,t} - C(a) - \frac{1-\rho^{N_{a,t}-C(a)+1}}{1-\rho} + 1 \right).$$

Taking expectation and letting $a \rightarrow \infty$ then gives the result. \square

4.2 SEMICIRCLE MICROSTRUCTURE

This section is devoted to computing the diffusivity of the channel system whose walls consist of a periodic focusing semicircle microscopic structure. The first subsection is devoted to a thorough analysis of the operator P for this geometry. We show that P is quasicompact and give an explicit formula for P for a certain range of pre-collision angles. The second subsection is devoted to the computation of \mathcal{D} using the method outlined in the above section.

4.2.1 A CLOSER LOOK AT P

To show that P is quasicompact we employ the technique of conditioning (see [16] and [17] for more details). The general idea of conditioning in this setting is to obtain a compact operator by considering P conditional on the event that trajectories satisfy a given property. As we will see, the compactness of this conditional operator will imply P is quasicompact.

Let Q denote the microscopic cell bounded by the semicircle and its diameter such that $\partial Q = \Gamma_0 \cup \Gamma_1$ where we renormalize so that the diameter Γ_0 is identified with $[0, 1]$ and Γ_1 is the semicircle with radius $1/2$. Let $\Psi_\theta(r) \in [0, \pi]$ denote the angle between the outgoing vector V and Γ_0 given that the trajectory enters Q with angle θ at position r .

We define a measurable partition of $M = I \times V = [0, 1] \times [0, \pi]$ as follows: let $M_1 \subset M$ be the subset of initial conditions whose billiard trajectories undergo exactly one or two collisions with ∂Q before returning to Γ_0 . Define P_1 as P conditional on the event M_1 , and similarly define P_2 from $M_2 = M \setminus M_1$. More precisely, if we let $M_j(\theta) = \{r \in I : (r, \theta) \in M_j\}$ and define $\alpha_j(\theta) = \lambda(M_j(\theta))$ for each $j = 1, 2$ and $\theta \in V$, then for each $f \in L^\infty(V, \mu)$, define

$$(P_j f)(\theta) = \begin{cases} \frac{1}{\alpha_j(\theta)} \int_{M_j(\theta)} f(\Psi_\theta(r)) dr, & \alpha_j(\theta) \neq 0 \\ 0, & \alpha_j(\theta) = 0. \end{cases}$$

We call P_j the *conditional operators* associated to the partition M_j . Note that it makes sense to write $Pf = \alpha_1 P_1 f + \alpha_2 P_2 f$. Let μ_j be the measure on V defined such that $d\mu_j = \frac{\alpha_j}{(\lambda \times \mu)(M_j)} d\mu$. It follows that P_j is self adjoint on $L^2(V, \mu_j)$.

Next note that P_1 has an integral kernel. Let $W_\theta^i = \{r \in I : (r, \theta) \in M_i\}$. Then W_θ^1 is the countable (or finite) union of open intervals $W_{\theta,j}$ for which the restriction $\Psi_{\theta,j} = \Psi_\theta|_{W_{\theta,j}}$ is a diffeomorphism from $W_{\theta,j}$ onto its image $V_{\theta,j}$. Define $\Gamma_\theta(\varphi) = \sum_j \chi_{V_{\theta,j}}(\varphi) \Lambda_{\theta,j}(\varphi)^{-1}$, where $\Lambda_{\theta,j}(\varphi) = \frac{1}{2} \left| \Psi'_\theta(\Psi_{\theta,j}^{-1}(\varphi)) \right| \sin \varphi$. Let

$$\omega_1(\theta, \varphi) = \frac{(\lambda \times \mu)(M_1) \Gamma_\theta(\varphi)}{\alpha_1(\theta) \alpha_1(\varphi)}.$$

It follows by way of change of variables that the operator P_1 on $L^2(V, \mu_1)$ is given by

$$(P_1 f)(\theta) = \int_V f(\varphi) \omega_1(\theta, \varphi) d\mu_1(\varphi).$$

To show P_1 is compact, it will suffice to show ω_1 is square integrable on $V \times V$. To this end, we first look at the function $\Psi_\theta(r)$. By the symmetry of the semicircle $\Psi_\theta(r)$ satisfies

$$\Psi_\theta(r) = \pi - \Psi_{\pi-\theta}(1-r).$$

It follows that it suffices to consider only $\theta \in (0, \pi/2)$.

Proposition 8. *The function $\Psi_\theta(r)$ has the following properties:*

1. *Let $\theta \in (0, \pi/2)$ and let $n \geq 1$ be the number of collisions a trajectory with initial data (r, θ) makes with the semicircle. Then*

$$\Psi_\theta(r) = \begin{cases} 2n \sin^{-1}((2r-1) \sin \theta) + n\pi - \theta, & r \in [0, 1/2] \\ 2n \sin^{-1}((2r-1) \sin \theta) - (n-2)\pi - \theta, & r \in (1/2, 1]. \end{cases}$$

2. *Let $\theta \in (\pi/4, \pi/2)$. Then $\Psi_\theta(r)$ has the following points of discontinuity in $[0, 1]$:*

$$r_0^{(n)} = \frac{1}{2} - \frac{\sin[(n\pi - \theta)/(2n+1)]}{2 \sin \theta}, \quad r_1^{(n)} = \frac{1}{2} + \frac{\sin[((n-1)\pi + \theta)/(2n+1)]}{2 \sin \theta},$$

$n \geq 1$.

3. Let $\theta \in (0, \pi/4)$. Then $\Psi_\theta(r)$ has only one point of discontinuity given by

$$r' = \frac{1}{2} + \frac{\sin \theta/3}{2 \sin \theta}.$$

We remark that if $\theta \in (0, \pi/4)$ then at most two collisions in the semicircle are possible and hence the formula in 1. is only valid for $n = 1, 2$. Further, we make more precise what is meant by the points of discontinuity given in 2. and 3. If $r \in (r_0^{(1)}, r_1^{(1)})$, then the initial conditions (r, θ) give a billiard trajectory which makes only one intermediary collision. And for $n \geq 2$, if $r \in (r_0^{(n)}, r_0^{(n-1)}) \cup (r_1^{(n-1)}, r_1^{(n)})$, then the initial conditions (r, θ) give a billiard trajectory which makes n intermediary collisions. For $0 < \theta < \pi/4$, the situation is simpler. The initial conditions (r, θ) for $r \in (0, r')$, give one intermediary collision, and for r in the complementary subinterval of I , there are two intermediary collisions. The proof of the proposition is by elementary trigonometry.

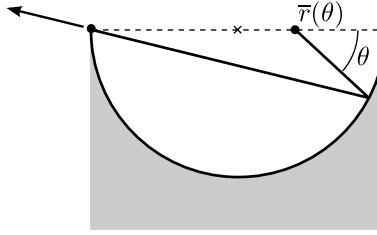


Figure 4.1: Definition of \bar{r} .

Proposition 9. The operator P_1 on $L^2(V, \mu_1)$ is compact.

Proof. As P_1 is given as an integral operator $(P_1 f)(\theta) = \int_V f(\varphi) \omega_1(\theta, \varphi) d\mu_1(\varphi)$ it suffices to show that $\omega_1 \in L^2(V \times V, \mu_1 \times \mu_1)$. By symmetry, we have the identity $\omega_1(\theta, \varphi) = \omega_1(\pi - \theta, \pi - \varphi)$ and the square of the L^2 -norm of ω_1 is

$$2 \int_0^{\pi/2} \int_V \omega_1^2(\theta, \varphi) d\mu_1(\varphi) d\mu_1(\theta).$$

Thus we show that the following two integrals are finite:

$$(4.1) \quad \int_0^{\pi/4} \int_V \omega_1^2(\theta, \varphi) d\mu_1(\varphi) d\mu_1(\theta), \quad \int_{\pi/4}^{\pi/2} \int_V \omega_1^2(\theta, \varphi) d\mu_1(\varphi) d\mu_1(\theta).$$

First consider the second integral. Let $\pi/4 < \theta < \pi/2$. Using the notation established in the previous proposition and further above, W_θ^1 is given by the single interval $W_{\theta,1} = (r_0^{(1)}, r_1^{(1)})$. Correspondingly, $V_{\theta,1} = (\pi/3 - \theta/3, \pi - \theta/3)$. Moreover, $\Psi_{\theta,1}(r) = \pi - \theta + 2 \sin^{-1}((2r - 1) \sin \theta)$. It follows that

$$|\Psi'_\theta(\Psi_{\theta,1}^{-1}(\varphi))| = \frac{4 \sin \theta}{\sin\left(\frac{\varphi + \theta}{2}\right)}$$

Now observe that

$$\begin{aligned} \int_{\pi/4}^{\pi/2} \int_V \omega_1^2(\theta, \varphi) d\mu_1(\varphi) d\mu_1(\theta) &= \int_{\pi/4}^{\pi/2} \int_V \frac{\Gamma_\theta(\varphi)^2}{\alpha_1(\theta)\alpha_1(\varphi)} d\mu(\varphi) d\mu(\theta) \\ &= \int_{\pi/4}^{\pi/2} \int_{V_{\theta,1}} \frac{\sin \theta}{\alpha_1(\theta)\alpha_1(\varphi)|\Psi'_\theta(\Psi_{\theta,1}^{-1}(\varphi))|^2 \sin \varphi} d\varphi d\theta. \end{aligned}$$

Now because θ, ϕ are bounded away from zero in the above integrals and because $\alpha_1(\theta) > 0$ for all θ , it follows that the above integral is finite.

We show that the first integral in (4.1) is finite. Let $0 < \theta < \pi/4$. Here W_θ^1 is given by the single interval $W_{\theta,1} = (0, r')$ and $V_{\theta,1} = (\pi - 3\theta, \pi - \theta/3)$. Moreover, $\Psi_{\theta,1}(r) = \pi - \theta + 2 \sin^{-1}((2r - 1) \sin \theta)$ as in the previous case. Hence $|\Psi'_\theta(\Psi_{\theta,1}^{-1}(\varphi))|$ is also as above. It follows that it suffices to show the following integral is finite:

$$\int_0^{\pi/4} \int_{\pi-3\theta}^{\pi-\theta/3} \frac{\sin^2\left(\frac{\varphi+\theta}{2}\right)}{\sin \theta \sin \varphi} d\varphi d\theta.$$

Note that for $\pi - 3\theta < \varphi < \pi - \theta/3$, we have $\varphi \geq \theta$, which implies $\sin\left(\frac{\varphi+\theta}{2}\right) \leq \sin^2 \varphi$. Therefore,

$$\begin{aligned} \int_0^{\pi/4} \int_{\pi-3\theta}^{\pi-\theta/3} \frac{\sin^2\left(\frac{\varphi+\theta}{2}\right)}{\sin \theta \sin \varphi} d\varphi d\theta &\leq \int_0^{\pi/4} \int_{\pi-3\theta}^{\pi-\theta/3} \frac{\sin \varphi}{\sin \theta} d\varphi d\theta \\ &= \int_0^{\pi/4} \int_{\theta/3}^{\pi-3\theta} 3\theta \frac{\sin \varphi}{\sin \theta} d\varphi d\theta \\ &\leq \int_0^{\pi/4} \frac{1}{\sin \theta} \left(\frac{(3\theta)^2 - (\theta/3)^2}{2} \right) d\theta, \end{aligned}$$

which is finite. \square

Having shown that P_1 is compact we are now ready to show that P is quasicompact. This is a consequence of the following general fact. (See Theorem 9.9 in [27].)

Proposition 10. *Let K and T be bounded self adjoint operators on a Hilbert space and suppose that K is compact. Then the essential spectrum of $T + K$ is contained in the essential spectrum of T . In particular, if $\|T + K\| = 1$ and $\|T\| < 1$, then the spectral gap $\gamma(T + K)$ of $T + K$ satisfies*

$$\gamma(T + K) \geq \min\{1 - \|T\|, \gamma(K)\}.$$

The quasicompactness of P then follows from letting $K = \alpha_1 P_1$ and $T = \alpha_2 P_2$ and noting that $1 - \|T\| \geq \inf \alpha_1 > 0$.

4.2.2 COMPUTATION OF \mathcal{D}

In this subsection we use the shorthand $Z_a := Z^{J(a)}$ and $Z_{a,j} := Z^{J(a)}(\Theta_j)$ where $J(a)$ is as given at the start of Section 4.1.

We show, for the example of Figure 2.2, that $\mathcal{D} = \frac{4rv}{\pi} \frac{1+\zeta}{1-\zeta}$ where $\zeta = -\frac{1}{4}\log 3$. Following the discussion in Section 4.1 we aim to compute

$$\lim_{a \rightarrow \infty} a^{-2} \sum_{0 < |i-j| < C(a)} \mathbb{E}[Z_{a,i} Z_{a,j}]$$

where we choose $C(a) = \log_3 \log a$. By stationarity, we are interested in computing $\mathbb{E}[Z_{a,0} Z_{a,j}]$ for $j < C(a)$. That is, we are interested in the first $C(a)$ collisions of trajectories with a shallow initial angle. Now although we've chosen these truncations of the between collision displacements because, as seen in the previous section, the transition probability kernel has a straightforward explicit formula for such pre-collision angles, they are not without their own complications. It's clear that to keep track of the trajectories whose j th displacement falls out of the truncation range, making $Z_{a,0} Z_{a,j}$ vanish, quickly becomes intractable. For this reason, we introduce the following so-called widened truncation, which, as we will show, will not change the diffusivity.

Consider a trajectory for which $Z_0 \in J(a)$. It follows that, for large enough a ,

$$|Z(3^j \Theta_0)| \leq |Z_j| \leq |Z(3^{-j} \Theta_0)|.$$

for all $j < C(a)$. A straightforward estimate then shows that

$$3^{-j} \exp(\log^\eta a) - C_1 < |Z_j| < 3^j a / \log^\gamma a + C_1$$

where $C_1 > 0$.

Define $K(a) := \{x : 3^{-C(a)} \exp(\log^\eta a) < |x| < 3^{C(a)} a / \log^\gamma a + C_1\}$. For the rest of the subsection we will consider the new truncated displacement $Z^{K(a)}$ as well as $Z^{J(a)}$, which we will continue to denote Z_a . Note that each $Z_j^{K(a)} = Z^{K(a)}(\Theta_j)$ is nonzero. Moreover, the following lemma shows that it suffices to compute $\mathbb{E}[Z_{a,i} Z_j^{K(a)}]$.

Lemma 8. *The following equality of limits holds:*

$$\lim_{a \rightarrow \infty} \sum_{0 < |i-j| < C(a)} a^{-2} \mathbb{E}[Z_{a,i} Z_{a,j}] = \lim_{a \rightarrow \infty} a^{-2} \sum_{0 < |i-j| < C(a)} \mathbb{E}[Z_{a,i} Z_j^{K(a)}]$$

Proof. Define $I_1 := \{x : 3^{-C(a)} \exp(\log^\eta a) < |x| < \exp(\log^\eta a)\}$ and $I_2 := \{x : a / \log^\gamma a < |x| < 3^{C(a)} a / \log^\gamma a + C_1\}$. Note that $K(a) = I_1(a) \cup I_2(a)$. Hence it suffices to show

$$\lim_{a \rightarrow \infty} a^{-2} \sum_{0 < |i-j| < C(a)} \mathbb{E}[Z_{a,i} (Z_j^{I_1(a)} + Z_j^{I_2(a)})] = 0.$$

Observe that

$$\begin{aligned} a^{-2} \left| \mathbb{E}[Z_{a,i} (Z_j^{I_1(a)} + Z_j^{I_2(a)})] \right| &\leq a^{-2} \mathbb{E}^{1/2}[Z_{a,i}^2] \left(\mathbb{E}^{1/2}[(Z_j^{I_1(a)})^2] + \mathbb{E}^{1/2}[(Z_j^{I_2(a)})^2] \right) \\ &= O(a^{-2} \log^{1/2} a (\log \log a)^{1/2}), \end{aligned}$$

where the last step is due to $\mathbb{E}[Z_{a,i}^2] = O(\log a)$ and $\mathbb{E}[(Z_j^{I_i(a)})^2] = O(\log \log a)$. Since the sum contains roughly $O(N_{a,t} C(a)) = O\left(\frac{a^2 \log \log a}{\log a}\right)$ such terms, the result follows. \square

Let $q_i = Z_i / Z_{i-1}$ for $i \geq 1$. The next lemma is a key technical tool in the computation.

Lemma 9. *Let $1 \leq j < O(|\log \theta|)$. Then $\mathbb{E}[q_1 \cdots q_j \mid \Theta_0 = \theta] = \zeta^j + AB^{j-1}\theta^2 + O(\theta^4)$ for constants A, B independent of θ .*

Proof. Observe that for θ sufficiently small, using the integral kernel for P derived in the previous subsection

$$\begin{aligned} \mathbb{E}[q_1 \mid \Theta_0 = \theta] &= \frac{1}{\cot \theta} \left(\int_{\pi-3\theta}^{\pi-\theta/3} \cot \varphi \frac{\cos\left(\frac{\varphi+\theta-\pi}{2}\right)}{4 \sin \theta} d\varphi + \int_{\theta/3}^{3\theta} \cot \varphi \frac{\cos\left(\frac{\varphi+\theta}{4}\right)}{8 \sin \theta} d\varphi \right) \\ &= \frac{1}{\cos \theta} \left(-\frac{1}{4} \int_{\theta/3}^{3\theta} \cot \varphi \cos\left(\frac{\varphi-\theta}{2}\right) d\varphi + \frac{1}{8} \int_{\theta/3}^{3\theta} \cot \varphi \cos\left(\frac{\varphi+\theta}{4}\right) d\varphi \right). \end{aligned}$$

One may check that

$$\frac{1}{\cos \theta} \int_{\theta/3}^{3\theta} \cot \varphi \cos\left(\frac{\varphi-\theta}{2}\right) d\varphi = 2 \log 3 + D_1 \theta^2 + O(\theta^4),$$

where D_1 is a constant, and likewise for the second integral above, albeit with a constant different from D_1 . The case $j = 1$ then follows.

Let $V_\theta = (\theta/3, 3\theta) \cup (\pi - 3\theta, \pi - \theta/3)$. Observe that

$$\begin{aligned} \mathbb{E}[q_1 q_2 \mid \Theta_0 = \theta] &= \mathbb{E}[\mathbb{E}[q_1 q_2 \mid \Theta_0 = \theta, \Theta_1 = \varphi] \mid \Theta_0 = \theta] = \int_{V_\theta} \mathbb{E}[q_1 q_2 \mid \Theta_0 = \theta, \Theta_1 = \varphi] P(\theta, d\varphi) \\ &= \int_{V_\theta} \frac{z(\varphi)}{z(\theta)} \mathbb{E}[q_2 \mid \Theta_0 = \theta, \Theta_1 = \varphi] P(\theta, d\varphi) = \int_{V_\theta} \frac{z(\varphi)}{z(\theta)} (\zeta + A\varphi^2 + O(\varphi^4)) P(\theta, d\varphi) \\ &= \zeta \mathbb{E}[q_1 \mid \Theta_0 = \theta] + \int_{V_\theta} \frac{z(\varphi)}{z(\theta)} (A\varphi^2 + O(\varphi^4)) P(\theta, d\varphi) \\ &= \zeta^2 + A\theta^2 + O(\theta^4) + \int_{V_\theta} \frac{z(\varphi)}{z(\theta)} (A\varphi^2 + O(\varphi^4)) P(\theta, d\varphi). \end{aligned}$$

Next, one may check that

$$\begin{aligned} \int_{V_\theta} \frac{z(\varphi)}{z(\theta)} (A\varphi^2 + O(\varphi^4)) P(\theta, d\varphi) &= \frac{1}{\cos \theta} \left(-\frac{1}{4} \int_{\theta/3}^{3\theta} \cot \varphi (A\varphi^2 + O(\varphi^4)) \cos\left(\frac{\varphi-\theta}{2}\right) d\varphi \right. \\ &\quad \left. + \frac{1}{8} \int_{\theta/3}^{3\theta} \cot \varphi (A\varphi^2 + O(\varphi^4)) \cos\left(\frac{\varphi+\theta}{4}\right) d\varphi \right) = AB\theta^2 + O(\theta^4) \end{aligned}$$

The case $j = 2$ follows. The rest of the argument follows by a similar induction argument. \square

With the above lemma in place we are ready to compute the correlations.

Lemma 10. *For $1 \leq j < C(a)$, $\mathbb{E}[Z_{a,0} Z_j^{K(a)}] = 4r^2 \zeta^j \Lambda(a) + AB^{j-1} \Gamma(a)$, where $\Lambda(a) \sim \log a$, $\Gamma(a) = O(\exp(-2 \log^\eta a))$, and A, B are the constants given in Lemma 9.*

Proof. Recall the interval $J(a) = \{x : \exp(\log^\eta a) < |x| < a/\log^\gamma a\}$. Observe that

$$\begin{aligned}\mathbb{E} \left[Z_{a,0} Z_j^{K(a)} \right] &= \int_0^\pi Z_a(\theta)^2 \mathbb{E}(q_1 \cdots q_j \mid \Theta_0 = \theta) \mu(d\theta) \\ &= 2 \int_0^\pi Z(\theta)^2 \mathbb{E}(q_1 \cdots q_j \mid \Theta_0 = \theta) \mathbb{1}_{J(a)} \mu(d\theta) \\ &= 2 \int_0^\pi Z(\theta)^2 \left(\zeta^j + AB^{j-1} \theta^2 + O(\theta^4) \right) \mathbb{1}_{J(a)} \mu(d\theta).\end{aligned}$$

We remark that because we are only considering here θ such that $\exp(\log^\eta a) < Z(\theta) < a/\log^\gamma a$, and hence $|\log \theta| < C \log a$ for some constant C , it follows that $j < C(a)$ is sufficiently small so that we may apply Lemma 9.

It is straightforward to compute $\int_0^\pi Z(\theta)^2 \mathbb{1}_{J(a)} \mu(d\theta) \sim 2r^2 \log a$. And moreover

$$\int_0^\pi Z(\theta)^2 O(\theta^2) \mathbb{1}_{J(a)} \mu(d\theta) = \int_0^\pi O(\theta) \mathbb{1}_{J(a)} d\theta = O((\exp(\log^\eta a))^{-2}).$$

The result now follows. \square

The summation of correlations is the final piece to our computation.

Proposition 11. *Let $U(a) = \sum_{0 < |i-j| < C(a)} \mathbb{E} \left[Z_{a,i} Z_j^{K(a)} \right]$. Then $\lim_{a \rightarrow \infty} a^{-2} U(a) = \frac{8trv}{\pi} \frac{\zeta}{1-\zeta}$.*

Proof. Observe that

$$\begin{aligned}U(a) &= 2 \left[(N_{a,t} - C(a) + 1) \sum_{i=1}^{C(a)-1} \mathbb{E} \left[Z_{a,0} Z_i^{K(a)} \right] + \sum_{i=1}^{C(a)-2} \sum_{j=1}^{C(a)-i-1} \mathbb{E} \left[Z_{a,0} Z_j^{K(a)} \right] \right] \\ &= 2 \left[(N_{a,t} - C(a) + 1) \sum_{i=1}^{C(a)-1} \left(4r^2 \zeta^i \Lambda(a) + AB^{i-1} \Gamma(a) \right) \right. \\ &\quad \left. + \sum_{i=1}^{C(a)-2} \sum_{j=1}^{C(a)-i-1} \left(4r^2 \zeta^j \Lambda(a) + AB^{j-1} \Gamma(a) \right) \right] \\ &= 2 \left[A \Gamma(a) \left((N_{a,t} - C(a) + 1) \frac{B^{C(a)} - B}{B(B-1)} + \frac{B^{C(a)} + B(C(a)-2) - B^2(C(a)-1)}{B(B-1)^2} \right) \right. \\ &\quad \left. + 4r^2 \Lambda(a) \left((N_{a,t} - C(a) + 1) \frac{\zeta^{C(a)} - \zeta}{\zeta - 1} + \frac{\zeta^{C(a)} + \zeta(C(a)-2) - \zeta^2(C(a)-1)}{(\zeta - 1)^2} \right) \right].\end{aligned}$$

Dividing by a^2 and letting $a \rightarrow \infty$ gives the result. \square

The value of \mathcal{D} then follows from adding the value from the proposition above to $4trv/\pi$ as discussed in Section 4.1.

4.3 PARAMETRIC FAMILIES

In this section we consider three different parametric families which are derived from the semicircle. Of primary interest will be how the diffusivity of the limiting process for each family changes as a function of the parameter.

We begin with the family formed by adding a middle wall of height h to the semicircle as shown in the figure above. Suppose $h < 1/2$; that is, the wall does not extend to the center of the semicircle. It is apparent by inspection that trajectories with a sufficiently small pre-collision angle will never, so to speak, notice the middle wall. And moreover, those trajectories with initial data (r, θ) that do notice the wall will behave like trajectories in the semicircle with no wall with initial data $(1-r, \pi - \theta)$ by symmetry. That is, if $\Psi_\theta^h(r)$ denotes the post-collision angle of a trajectory with initial data (r, θ) in the middle wall geometry and similarly $\Psi_\theta(r) = \Psi_\theta^0(r)$, then $\Psi_\theta^h(r) = \Psi_{\pi-\theta}(1-r)$ for initial conditions (r, θ) for which the trajectory hits the middle wall. It follows that the operator P_h for the middle wall geometry is quasicompact. Moreover, as pointed out earlier, the diffusivity \mathcal{D}_h for P_h depends only on trajectories with arbitrarily shallow angles by the formula in Proposition 7. It follows that the diffusivity $\mathcal{D}(h)$ is constant and equal to the diffusivity for the semicircle with no wall for all $h < 1/2$.

Further, using the symmetry $\Psi_\theta^h(r) = \Psi_{\pi-\theta}(1-r)$ and following the proof given for the semicircle, the diffusivity $\mathcal{D}(1/2)$ for the geometry with a middle that extends exactly to the center of the semicircle is given by $\mathcal{D}(1/2) = \frac{4rv}{\pi} \frac{1-\zeta}{1+\zeta}$ where $\zeta = -\frac{1}{4} \log 3$ as in the semicircle. We summarize these facts as follows.

Proposition 12. *For the middle wall modification of the semicircle with middle wall height h , $\mathcal{D}(h) = \mathcal{D}$, for $h < 1/2$, where \mathcal{D} is the diffusivity for the semicircle with no wall, and for $h = 1/2$ the diffusivity is given by*

$$\mathcal{D}(1/2) = \frac{4rv}{\pi} \frac{1-\zeta}{1+\zeta},$$

where $\zeta = -1/4 \log 3$.

It is interesting to note that the diffusivity is not a continuous function of the parameter. We also remark that the case $h > 1/2$ when the middle wall extends outside the semicircle requires a different analysis altogether, which we leave for a future paper.

Next we look to the geometry formed by splitting the semicircle and adding a flat bottom of length $h \in (0, 1)$ as shown above. We renormalize the size of the semicircles so that they have radius $(1-h)/2$. We also establish the notation $a = (1+h)/2$, $b = (1-h)/2$. While qualitatively similar to the semicircle, the angle function $\Psi_\theta^h(r)$ requires a new detailed analysis, which we sketch here.

We begin by noting that by symmetry it again suffices to consider only pre-collision angles $\theta \in (0, \pi/2)$. And moreover, for sufficiently small pre-collision angles θ at most two intermediary collisions are possible within the cell. In the discussion that follows we consider only such θ . Let $r' \in (0, 1)$ be the point of entry for which $\Psi_\theta^h(r)$ is discontinuous. That is, r' is chosen such that trajectories with initial data (r, θ) for $r \in (0, r')$ experience one intermediary collision, and for those with $r \in (r', 1)$, there are two intermediary collisions. It follows that $\Psi_\theta^h(r) = \pi - \theta - 2\beta_1(r)$ for $r \in (0, r')$ where $\beta_1 = \beta_1(r)$ satisfies $b \sin \beta_1 = (a-r) \sin \theta$. We may also characterize r' as the value of r that satisfies $a \sin(\theta - 2\beta_1) = b \sin \beta_1$. From these observations it follows that

$$\Psi_\theta^h(0) = \pi - \frac{3+h}{1-h} \theta + O(\theta^3), \quad \lim_{r \rightarrow (r')^-} \Psi_\theta^h(r) = \pi - \frac{1-h}{3+h} \theta + O(\theta^3).$$

Following the notation established in the discussion on the semicircle,

$$V_{\theta,1} = \left[\pi - \frac{3+h}{1-h} \theta + O(\theta^3), \pi - \frac{1-h}{3+h} \theta + O(\theta^3) \right].$$

Moreover, if we let $\Theta = \Psi_\theta(r)$ it follows from implicit differentiation that

$$\Theta'(r) = \frac{1}{1-h} \frac{4 \sin \theta}{\cos\left(\frac{\Theta+\theta-\pi}{2}\right)}$$

which is the corresponding value in the semicircle case except for the factor of $(1-h)^{-1}$.

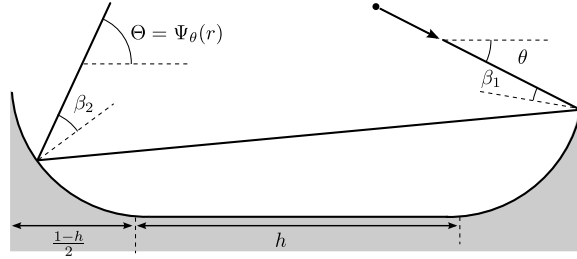


Figure 4.2:

For $r \in (r', 1)$, we have $\Psi_\theta^h(r) = 2\beta_1(r) + 2\beta_2(r) - \theta$, where $\beta_1(r)$ is as above and $\beta_2 = \beta_2(r)$ satisfies $b \sin \beta_2 = h \sin(2\beta_1 - \theta) + \sin \beta_1$. It follows by symmetry that

$$V_{\theta,2} = \left[\frac{1-h}{3+h} \theta + O(\theta^3), \frac{3+h}{1-h} \theta + O(\theta^3) \right].$$

Further, by implicit differentiation again

$$\Theta'(r) = \frac{1+h}{(1-h)^2} \frac{8 \sin \theta}{\cos\left(\frac{\Theta+\theta}{4}\right)},$$

which again resembles the semicircle case but for the factor of $(1+h)(1-h)^{-2}$. As in the computation of the diffusivity for the semicircle we find the following.

Proposition 13. *For the flat bottom of length $h \in (0, 1)$ modification of the semicircle, we have the following value of diffusivity as a function of h :*

$$\mathcal{D}(h) = \frac{4rv}{\pi} \frac{1+\zeta_h}{1-\zeta_h},$$

where

$$\zeta_h = -\frac{1+3h}{4} \frac{1-h}{1+h} \log \frac{3+h}{1-h}.$$

Notice that the limiting case $h = 0$ gives the diffusivity of the semicircle while $h = 1$ gives $\zeta_h = 0$ which gives the diffusivity in the case that at each post-collision angle is chosen independently according to the distribution μ .

The final family of interest is formed by adding a flat side of length $h \in (0, 1)$ between semicircles as shown above. The key observation here is that the operator P_h corresponding to

such a geometry can be thought of as a sum of conditional operators given by $P_h = (1-h)P + hI$ where P is the operator corresponding to the semicircle geometry and I is the identity operator. Such an operator is a generalized Maxwell-Smoluchowski model as discussed in the introduction. Next notice that since P and I commute the spectra of P_h and P are the same, and in fact every spectral value of P_h is given by $(1-h)\lambda + h$ for some unique spectral value λ of P . It follows that

$$\int_{-1}^1 \frac{1+\lambda}{1-\lambda} \Pi_a^h(d\lambda) = \int_{-1}^1 \frac{1+(1-h)\lambda+h}{1-(1-h)\lambda-h} \Pi_a(d\lambda) = \int_{-1}^1 \left(\frac{1}{1-h} \frac{1+\lambda}{1-\lambda} + \frac{h}{1-h} \right) \Pi_a(d\lambda),$$

where Π_a is the spectral measure as given in the statement of Theorem 2, and similarly Π_a^h is derived from the projection valued measure Π^h associated to P_h given by the spectral theorem. The following proposition then follows from the discussion above and the spectral formulation of the diffusivity.

Proposition 14. *For the flat top of length $h \in (0, 1)$ modification of the semicircle, we have the following value of diffusivity as a function of h :*

$$\mathcal{D}(h) = \frac{1}{1-h} \mathcal{D} + \frac{h}{1-h} \frac{4r\nu}{\pi} = \frac{4r\nu}{\pi(1-h)} \left(h + \frac{1+\zeta}{1-\zeta} \right),$$

where \mathcal{D} is the diffusivity for the unmodified semicircle and $\zeta = -1/4 \log 3$.

5 ADDITIONAL PROOFS

We collect here proofs of some of the more technical propositions and lemmas from earlier parts of the paper.

5.1 SKETCH OF PROOF OF PROPOSITION 2

The proposition results from tedious but elementary and straightforward integrations. We show a few steps to convey the flavor.

By identifying the tangent space to \mathbb{C} at $q \in \partial\mathbb{C}$ with $\mathbb{R}^k \oplus \mathbb{R}^{n-k}$, the unit normal vector n is identified with $e_n = (0, \dots, 0, 1)$ and \mathbb{H}_q is identified with the half-space consisting of vectors $v = (v_1, v_2) \in \mathbb{R}^k \oplus \mathbb{R}^{n-k}$ such that $\langle v, e_n \rangle > 0$. For such a post-collision velocity v , the point of next collision with the channel boundary is $q + \tau v$, where $\tau_b = 2r \langle v, e_n \rangle / |v_2|^2$ is the time interval between the two collisions and $Z(v) = 2r \langle v, e_n \rangle v_1 / |v_2|^2$ is the between-collisions displacement vector in “horizontal” factor \mathbb{R}^k as represented in Figure 2.1. We assume that v has the following general form:

$$dv(v) = C \langle v, n \rangle f(|v|^2) dV(v),$$

in which $f(x)$ is a nonnegative function on $[0, \infty)$ such that $\int_0^\infty x^n f(x^2) dx < \infty$. We allow f to be distributional (a delta-measure concentrated on a fixed value of $|v|$) so as to include the case where v is supported on an hemisphere. Let $S_+ := S_+^{n-1}$ be the unit hemisphere in \mathbb{H} . Then \mathbb{H} is diffeomorphic to $S_+ \times (0, \infty)$ under polar coordinates $v \mapsto (w, \rho)$, where $w = v/|v|$

and $\rho = |v|$, and $dV(v) = \rho^{n-1} dV_{\text{sph}}(w) d\rho$. Also define the notations $S_{+a} := S_+ \cap \mathbb{H}(a)$ and $E(a) := E_v[|Z|^2, \mathbb{H}(a)]$. Then

$$E(a) = C \int_0^\infty \int_{S_{+a}} \rho^n f(\rho^2) |Z(w)|^2 \langle w, n \rangle dV_{\text{sph}}(w) d\rho = C' \int_{S_{+a}} |Z(w)|^2 \langle w, n \rangle dV_{\text{sph}}(w),$$

where we have used that $Z(v) = Z(w)$. Here and below, C, C', C'' are positive constants that can be obtained explicitly.

The image of S_{+a} under the projection map $\pi : w \in S_+ \mapsto \overline{w} \in \mathbb{B}^{n-1}$ contains the ball \mathbb{B}_a^{n-1} of radius $(1 + (2/a)^2)^{-1/2}$, and it is equal to \mathbb{B}_a^{n-1} when $n - k = 1$. The volume elements dV_{sph} on the hemisphere and dV_{n-1} on the ball are related under π by $\langle w, n \rangle dV_{\text{sph}}(w) = dV_{n-1}(\overline{w})$. Also let $x_1 = \pi_1(x)$ be the natural projection from the unit ball in \mathbb{R}^{n-1} to the unit ball \mathbb{B}^k in the horizontal factor \mathbb{R}^k , and $x_2 = \pi_2(x)$ the projection to the complementary factor \mathbb{R}^{n-k-1} in \mathbb{R}^{n-1} . Then the limit as $a \rightarrow \infty$ of $\int_{S_{+a}} |Z(w)|^2 \langle w, n \rangle dV_{\text{sph}}(w)$ is, up to multiplicative positive constant, the same as the limit of

$$\begin{aligned} \int_{\mathbb{B}_a^{n-1}} \frac{(1 - |x_1|^2 - |x_2|^2) |x_1|^2}{(1 - |x_1|^2)^2} dV_{n-1}(x) &= \int_{\mathbb{B}_a^k} \int_{\mathbb{B}_{|x_1|}^{n-k-1}} \frac{|x_1|^2 (1 - |x_1|^2 - |x_2|^2)}{(1 - |x_1|^2)^2} dV_{n-k-1}(x_2) dV_k(z_1) \\ &= \frac{2\text{Vol}(\mathbb{B}^{n-k-1})}{n-k+1} \int_{\mathbb{B}_e^k} |x_1|^2 (1 - |x_1|^2)^{\frac{n-k-3}{2}} dV_k(x_1) \\ &= \frac{k}{n-k+1} \text{Vol}(\mathbb{B}^{n-k-1}) \text{Vol}(\mathbb{B}^k) \int_0^{\frac{a^2}{4+a^2}} s^{\frac{k}{2}} (1-s)^{\frac{n-k-3}{2}} ds \end{aligned}$$

where the iterated integrals were carried out in polar coordinates, in which volume elements are related by $dV_n(v) = |v|^{n-1} dV_{\text{sph}}(v/|v|) d|v|$. The limit of the remaining integral, as a goes to ∞ , is a Beta-function of the exponents of s in the integrand; it, and the volumes of unit balls, can be written in terms of Gamma-functions and further simplified.

The expected values of $\tau_b(v) = 2r \langle v, n \rangle / |v_2|^2$ are shown by similar computations to take the form

$$E_\mu[\tau_b] = \frac{2r}{s} \frac{\Gamma(\frac{n+1}{2})}{\pi^{\frac{n-1}{2}}} I(n, k), \quad E_{\mu_\beta}[\tau_b] = r (2\beta M)^{\frac{1}{2}} \frac{\Gamma(\frac{n}{2})}{\pi^{\frac{n-1}{2}}} I(n, k),$$

where s is the speed (or radius) of the hemisphere on which μ is supported and

$$I(n, k) := \int_{S_+} \frac{\langle x, n \rangle^2}{|x_2|^2} dV_{\text{sph}}(x) = \frac{\pi^{\frac{n}{2}}}{(n-k)\Gamma(\frac{n}{2})},$$

S_+ being the hemisphere of radius 1 in \mathbb{H} .

Finally, observed that $\mathbb{E}_v[(Z_a^u)^2] = \mathbb{E}_v[|Z_a|^2]/k$ since v is rotationally symmetric in the \mathbb{R}^k subspace. The proposition is now a consequence of these observations.

5.2 PROOFS OF CLT LEMMAS

Proof of Lemma 2. We again employ the notation $D_k^l := \sum_{j=k}^{l-1} Z_{a,j} - \sum_{j=k}^{n_{a,t}-1} Z_{a,t}$. Since $\sum_{j=0}^{N_{a,t}-1} Z_{a,j} = \sum_{j=0}^{n_{a,t}-1} Z_{a,j} + D_0^{N_{a,t}}$ it suffices to show $D_0^{N_{a,t}} \rightarrow 0$ in probability. Before getting to this directly, we begin with a few technical remarks to be used in what follows.

Let $v > 1$ and define

$$n_1 = \left\lfloor \left(1 - \frac{\epsilon^{2v}}{2}\right) n_{a,t} \right\rfloor + 1, \quad n_2 = \left\lfloor \left(1 + \frac{\epsilon^{2v}}{2}\right) n_{a,t} \right\rfloor - 1.$$

Then $\mathbb{P}(n_1 \leq N_{a,t} \leq n_2) \geq 1 - \epsilon$ for a large enough. Let $a^* = \epsilon^v a$, $n_{a,t}^* = n_{a^*,t}$. Observe that

$$\epsilon^{2v} n_{a,t} \leq \epsilon^{2v} \frac{ah(a)t}{\mathbb{E}[\tau_b]} \leq \frac{a^* h(a^*)t}{\mathbb{E}[\tau_b]} \leq n_{a,t}^* + 1.$$

Therefore, $n_2 - n_1 \leq \epsilon^{2v} n_{a,t} - 1 \leq n_{a,t}^*$. We are now ready to address the convergence in probability. Observe that

$$\begin{aligned} \mathbb{P}\left(\left|D_1^{N_{a,t}}\right| > a\epsilon\right) &= \sum_{j=1}^{\infty} \mathbb{P}\left(N_{a,t} = j, \left|D_1^{N_{a,t}}\right| > a\epsilon\right) \\ &= \sum_{j=n_1}^{n_2} \mathbb{P}\left(N_{a,t} = j, \left|D_1^{N_{a,t}}\right| > a\epsilon\right) + \sum_{j \notin [n_1, n_2]} \mathbb{P}\left(N_{a,t} = j, \left|D_1^{N_{a,t}}\right| > a\epsilon\right) \end{aligned}$$

Notice for the second term above that

$$\sum_{j \notin [n_1, n_2]} \mathbb{P}\left(N_{a,t} = j, \left|D_1^{N_{a,t}}\right| > a\epsilon\right) \leq \sum_{j \notin [n_1, n_2]} \mathbb{P}\left(N_{a,t} = j\right) = 1 - \mathbb{P}(n_1 \leq N_{a,t} \leq n_2) \leq \epsilon.$$

For the first term observe that

$$\sum_{j=n_1}^{n_2} \mathbb{P}\left(N_{a,t} = j, \left|D_1^{N_{a,t}}\right| > a\epsilon\right) \leq \sum_{j=n_1}^{n_2} \mathbb{P}\left(N_{a,t} = j, \max_{n_1 \leq k \leq n_2} \left|D_1^k\right| > a\epsilon\right) \leq \mathbb{P}\left(\max_{n_1 \leq k \leq n_2} \left|D_1^k\right| > a\epsilon\right).$$

And notice that

$$\begin{aligned} \mathbb{P}\left(\max_{n_{a,t} < k \leq n_2} \left|D_1^k\right| > a\epsilon\right) &= \mathbb{P}\left(\max_{n_{a,t} < k \leq n_2} \left|\sum_{i=n_{a,t}+1}^k Z_{a,i}\right| > a\epsilon\right) \\ &= \mathbb{P}\left(\max_{1 \leq k \leq n_2 - n_{a,t}} \left|\sum_{i=1}^k Z_{a,i}\right| > a\epsilon\right) \leq \mathbb{P}\left(\max_{1 \leq k \leq n_2 - n_1} \left|\sum_{i=1}^k Z_{a,i}\right| > a\epsilon\right). \end{aligned}$$

Similarly,

$$\mathbb{P}\left(\max_{n_1 \leq k < n_{a,t}} \left|D_1^k\right| > a\epsilon\right) \leq \mathbb{P}\left(\max_{1 \leq k \leq n_2 - n_1} \left|\sum_{i=1}^k Z_{a,i}\right| > a\epsilon\right).$$

It then follows that

$$\mathbb{P}\left(\max_{n_1 \leq k \leq n_2} \left|D_1^k\right| > a\epsilon\right) \leq 2\mathbb{P}\left(\max_{1 \leq k \leq n_2 - n_1} \left|\sum_{i=1}^k Z_{a,i}\right| > a\epsilon\right) \leq 2\mathbb{P}\left(\max_{1 \leq k \leq n_{a,t}^*} \left|\sum_{i=1}^k Z_{a,i}\right| > a\epsilon\right).$$

Next observe that by the symmetry of $Z_{a,i}$,

$$\frac{\mathbb{P}\left(\left|\sum_{i=1}^{n_{a,t}^*} Z_{a,i}\right| > a\epsilon, \max_{1 \leq k \leq n_{a,t}^*} \left|\sum_{i=1}^k Z_{a,i}\right| > a\epsilon\right)}{\mathbb{P}\left(\max_{1 \leq k \leq n_{a,t}^*} \left|\sum_{i=1}^k Z_{a,i}\right| > a\epsilon\right)} = \mathbb{P}\left(\left|\sum_{i=1}^{n_{a,t}^*} Z_{a,i}\right| > a\epsilon \mid \max_{1 \leq k \leq n_{a,t}^*} \left|\sum_{i=1}^k Z_{a,i}\right| > a\epsilon\right) \geq \frac{1}{2},$$

which implies

$$\mathbb{P}\left(\max_{1 \leq k \leq n_{a,t}^*} \left| \sum_{i=1}^k Z_{a,i} \right| > a\epsilon\right) \leq 2\mathbb{P}\left(\left| \sum_{i=1}^{n_{a,t}^*} Z_{a,i} \right| > a\epsilon, \max_{1 \leq k \leq n_{a,t}^*} \left| \sum_{i=1}^k Z_{a,i} \right| > a\epsilon\right) \leq 2\mathbb{P}\left(\left| \sum_{i=1}^{n_{a,t}^*} Z_{a,i} \right| > a\epsilon\right).$$

We summarize and observe that by assumption

$$\begin{aligned} \sum_{j=n_1}^{n_2} \mathbb{P}\left(N_{a,t} = j, \left| D_1^{N_{a,t}} \right| > a\epsilon\right) &\leq 4\mathbb{P}\left(\left| \sum_{i=1}^{n_{a,t}^*} Z_{a,i} \right| > a\epsilon\right) = 4\mathbb{P}\left(\left| \sum_{i=1}^{n_{a,t}^*} Z_{a,i} \right| > a^* \epsilon^{1-\nu}\right) \\ &\rightarrow \frac{8}{\sqrt{2\pi t^D}} \int_{\epsilon^{1-\nu}}^{\infty} e^{-x^2/2t^D} dx, \end{aligned}$$

as $a \rightarrow \infty$. In letting $\epsilon \rightarrow 0$ the last line above vanishes. \square

Proof of Lemma 3. Let $I_1(a) := \{x : a/\log^Y(a) < |x| < a \log \log a\}$ and $I_2 := \{x : |x| > a \log \log a\}$. It will suffice to show that each of the sums $\sum_{j=0}^{N_{a,t}-1} a^{-1} Z_j^{I_i(a)}$ for $i = 1, 2$ converges to zero in probability.

We first consider the truncation by I_2 . As there is no ambiguity, we use the shorthand $Z_a := Z^{I_2}$ and $Z_{a,j} = Z^{I_2}(\Theta_j)$. Let $\epsilon > 0$ and observe that

$$\begin{aligned} \mathbb{P}\left(\left| \sum_{j=0}^{N_{a,t}-1} Z_{a,j} \right| > a\epsilon\right) &\leq \mathbb{P}\left(\sum_{j=0}^{N_{a,t}-1} |Z_{a,j}| > a\epsilon\right) = \sum_{N=1}^{\infty} \mathbb{P}\left(\sum_{j=0}^N |Z_{a,j}| > a\epsilon\right) \mathbb{P}(N_{a,t} = N) \\ &\leq \sum_{N=1}^{\infty} \mathbb{P}(Z_j \in I_2 \text{ for some } j, 0 \leq j \leq N-1) \mathbb{P}(N_{a,t} = N) \\ &\leq \sum_{N=1}^{\infty} \sum_{j=0}^{N-1} \mathbb{P}(Z_j \in I_2) \mathbb{P}(N_{a,t} = N) \\ &= \mathbb{E}[N_{a,t}] \mathbb{P}(Z_0 \in I_2). \end{aligned}$$

Next note that

$$\begin{aligned} \mathbb{P}(Z_0 \in I_2) &= \int_0^{\cot^{-1}(a \log \log a / (2r))} \sin \theta d\theta \\ &= 1 - \cos(\cot^{-1}(a \log \log a / (2r))) = O((a \log \log a)^{-2}). \end{aligned}$$

Moreover, a straightforward application of Lemma 1 and the dominated convergence theorem shows that $\mathbb{E}[N_{a,t}] = O(ah(a))$. It follows that

$$\mathbb{P}\left(\left| \sum_{j=0}^{N_{a,t}-1} Z_{a,j} \right| > a\epsilon\right) \leq O\left(\frac{1}{\log a \cdot (\log \log a)^2}\right) \rightarrow 0$$

as $a \rightarrow \infty$.

Next we consider the truncation by I_1 . As before we use the shorthand $Z_a := Z^{I_1}$. To show that the sum $\sum_{j=0}^{N_{a,t}-1} a^{-1} Z_{a,j}$ converges to zero in probability, we use Chebyshev's inequality.

To this end, observe that as in the proof of Theorem 1

$$\mathbb{E} \left[\left(\sum_{j=0}^{N_{a,t}-1} a^{-1} Z_{a,j} \right)^2 \right] = \int_{-1}^1 \frac{1+\lambda}{1-\lambda} \frac{\mathbb{E}[N_{a,t} + O(1)]}{ah(a)} \frac{h(a)}{a} \|Z_a\|^2 \Pi_a(d\lambda),$$

where we recall $\Pi_a = \|Z_a\|^{-2} \langle Z_a, \Pi(d\lambda) Z_a \rangle$ is the spectral measure associated to Z_a . Note $\|Z_a\|^2 = O(\log \log a)$ and $h(a)/a = 1/\log a$, while all other factors in the integrand are bounded as $a \rightarrow \infty$. The result follows. \square

Proof of Lemma 4. Because of the slight difference in definitions, we show separately that $\sum_{i=1}^{k_{a,t}-1} V_{a,i} \rightarrow 0$ and $V_{a,k_{a,t}} \rightarrow 0$. To prove each of these, note that by Chebyshev's inequality, it suffices to show

$$\mathbb{E} \left[\left(\sum_{i=1}^{k_{a,t}-1} V_{a,i} \right)^2 \right] \rightarrow 0, \quad \mathbb{E} [V_{a,k_{a,t}}^2] \rightarrow 0,$$

respectively. We start with the first. Observe that

$$\mathbb{E} \left[\left(\sum_{i=1}^{k_{a,t}-1} V_{a,i} \right)^2 \right] = k_{a,t} \mathbb{E} [V_{a,1}^2] + 2 \sum_{1 \leq i < j \leq k_{a,t}-1} \mathbb{E} [V_{a,i} V_{a,j}]$$

and

$$\mathbb{E} [V_{a,1}^2] = \mathbb{E} \left[\left(\sum_{j=0}^{s_{a,t}-1} a^{-1} Z_{a,j} \right)^2 \right] = \int_{\sigma} \frac{1+\lambda}{1-\lambda} \frac{s_{a,t} + O(1)}{ah(a)} \frac{h(a)}{a} \|Z_a\|^2 \Pi_a(d\lambda) = O((ah(a))^{\alpha-1}).$$

Therefore, $k_{a,t} \mathbb{E} [V_{a,1}^2] = O((ah(a))^{\alpha-\beta}) \rightarrow 0$. The number of terms in $\sum_{1 \leq i < j \leq k_{a,t}-1} V_{a,i} V_{a,j}$ is $(k_{a,t}-1)(k_{a,t}-2)$ and each term $V_{a,i} V_{a,j}$ itself contains $s_{a,t}^2$ terms of the form $a^{-2} Z_{a,m} Z_{a,n}$. It follows that

$$2 \sum_{1 \leq i < j \leq k_{a,t}-1} \mathbb{E} [V_{a,i} V_{a,j}] = O((ah(a))^{2(1-\beta)+2\alpha-1}) \rightarrow 0.$$

Finally, the sum in $V_{a,k_{a,t}}$ contains by definition less than $b_{a,t} + s_{a,t}$ terms. Just as above, it follows that $\mathbb{E} [V_{a,k_{a,t}}^2] \leq O((ah(a))^{\beta-1}) \rightarrow 0$. \square

Proof of Lemma 5. Let $w_i = \exp(i\mu U_{a,i})$ for $1 \leq i \leq k_{a,t}$. Also let $\sigma_{w_i}^2 = \mathbb{E} [w_i^2] - \mathbb{E}^2 [w_i]$. Define $\mathcal{E}(w_1, w_2) := \mathbb{E} [w_1 w_2] - \mathbb{E} [w_1] \mathbb{E} [w_2]$. Because of the small block gap of size $s_{a,t}$ between big blocks, $|\mathcal{E}(w_1, w_2)| = |\sigma_{w_1} \sigma_{w_2} \text{corr}(w_1, w_2)| \leq 4 |\text{corr}(w_1, w_2)| \leq 4 |\rho(s_{a,t})|$. Moreover,

$$\begin{aligned} |\mathbb{E} [w_1 w_2 w_3] - \mathbb{E} [w_1] \mathbb{E} [w_2] \mathbb{E} [w_3]| &\leq |\mathcal{E}(w_1, w_2 w_3)| + |\mathbb{E} [w_1] \mathcal{E}(w_2, w_3)| \\ &= |\sigma_{w_1} \sigma_{w_2 w_3} \text{corr}(w_1, w_2 w_3)| + |\mathbb{E} [w_1] \mathcal{E}(w_2, w_3)| \\ &\leq 4 |\rho(s_{a,t})| + 4 |\rho(s_{a,t})|. \end{aligned}$$

It then follows by induction that

$$\left| \mathbb{E} \left[\exp \left(i\mu \sum_{i=1}^{k_{a,t}} U_{a,i} \right) \right] - \prod_{i=1}^{k_{a,t}} \mathbb{E} [\exp(i\mu U_{a,i})] \right| \leq 4k_{a,t} |\rho(s_{a,t})| \rightarrow 0$$

as $a \rightarrow \infty$. \square

Proof of Lemma 6. A simple induction argument shows that if $z_1, \dots, z_m, w_1, \dots, w_m \in \mathbb{C}$ are of modulus at most 1, then

$$\left| \prod_{i=1}^m z_i - \prod_{i=1}^m w_i \right| \leq \sum_{i=1}^m |z_i - w_i|.$$

Applying the remark to $|\mathbb{E}[\exp(i\mu U_{a,i})]|$ and, for large enough a , $\left|1 - \frac{\mu^2}{2k_{a,t}} t\mathcal{D}\right|$, we see

$$\begin{aligned} \left| \prod_{i=1}^{k_{a,t}} \mathbb{E}[\exp(i\mu U_{a,i})] - \left(1 - \frac{\mu^2}{2k_{a,t}} t\mathcal{D}\right)^{k_{a,t}} \right| &\leq \sum_{i=1}^{k_{a,t}} \left| \mathbb{E}[\exp(i\mu U_{a,i})] - \left(1 - \frac{\mu^2}{2k_{a,t}} t\mathcal{D}\right) \right| \\ &= k_{a,t} \left| \mathbb{E}[\exp(i\mu U_{a,1})] - \left(1 - \frac{\mu^2}{2k_{a,t}} t\mathcal{D}\right) \right| \\ &= k_{a,t} \left| 1 - \frac{\mu^2}{2} \mathbb{E}[U_{a,1}^2] + O(\mathbb{E}[U_{a,1}^3]) - \left(1 - \frac{\mu^2}{2k_{a,t}} t\mathcal{D}\right) \right| \\ &\leq \frac{\mu^2}{2} |k_{a,t} \mathbb{E}[U_{a,1}^2] - t\mathcal{D}| + |k_{a,t} O(\mathbb{E}[U_{a,1}^3])|. \end{aligned}$$

Now, it follows from the spectral representation of \mathcal{D} that $|k_{a,t} \mathbb{E}[U_{a,1}^2] - t\mathcal{D}| \rightarrow 0$.

Expanding $U_{a,1}^3$ results in $b_{a,t}^3$ terms of the form $a^{-3} Z_{a,i} Z_{a,j} Z_{a,k}$. Suppose $i \leq j \leq k$ and let $D_1 = j - i$ and $D_2 = k - j$. Let $C(a) = C \log a$, where $C > 4\beta$. We separate the terms in the expansion of $U_{a,1}^3$ into one group containing those terms whose indices satisfy $D_1 \leq C(a)$ and $D_2 \leq C(a)$; and another group with those terms for which $D_1 > C(a)$ or $D_2 > C(a)$. Suppose $Z_{a,i} Z_{a,j} Z_{a,k}$ is in the first group. Then

$$\mathbb{E}[Z_{a,i} Z_{a,j} Z_{a,k}] \leq \mathbb{E}^{1/3}[|Z_{a,i}|^3] \mathbb{E}^{1/3}[|Z_{a,j}|^3] \mathbb{E}^{1/3}[|Z_{a,k}|^3] = \mathbb{E}[|Z_{a,i}|^3] = O(a/\log^\gamma a).$$

Moreover, of the $b_{a,t}^3$ total terms, $O(b_{a,t} C(a)^2)$ of them fall into this first group. Thus the contribution of these terms to $|k_{a,t} O(\mathbb{E}[U_{a,1}^3])|$ is at most of the order $O(\log^{1-\gamma} a)$ which is negligible as $a \rightarrow \infty$.

Suppose next that $Z_{a,i} Z_{a,j} Z_{a,k}$ is in the second group and assume without loss of generality that $D_1 > C(a)$. Observe that

$$\mathbb{E}[Z_{a,i} Z_{a,j} Z_{a,k}] = \text{corr}(Z_{a,i}, Z_{a,j} Z_{a,k}) \mathbb{E}^{1/2}[Z_{a,i}^2] \left(\mathbb{E}[(Z_{a,j} Z_{a,k})^2] - \mathbb{E}^2[Z_{a,j} Z_{a,k}] \right)^{1/2}.$$

Recall that $\mathbb{E}[Z_{a,i}^2] = O(\log a)$. Moreover, by the Cauchy-Schwarz inequality, stationarity, and further direct computation of moments

$$\mathbb{E}[(Z_{a,j} Z_{a,k})^2] \leq \mathbb{E}[Z_{a,i}^4] = O(a^2 / \log^{2\gamma} a) \text{ and } \mathbb{E}^2[Z_{a,j} Z_{a,k}] \leq \mathbb{E}^2[Z_{a,j}^2] = O(\log^2 a).$$

Finally, using the mixing properties of the process $\text{corr}(Z_{a,i}, Z_{a,j} Z_{a,k}) \leq \rho(C(a)) = O(a^{-C})$. Putting these three estimates together, we see that

$$a^{-3} \mathbb{E}[Z_{a,i} Z_{a,j} Z_{a,k}] \leq O(a^{-(C+2)} \log^{1/2-\gamma} a)$$

Since, $O(b_{a,t}^3 - b_{a,t} C(a)^2) = O(b_{a,t}^3) = O(a^{6\beta} \log^{-3\beta} a)$ terms are in this second group, their contribution to $|k_{a,t} O(\mathbb{E}[U_{a,1}^3])|$ will be of order at most $O(a^{4\beta-C} \log^{-1/2-2\beta-\gamma} a)$, which is indeed negligible with our choice of C . The lemma now follows. \square

REFERENCES

- [1] O. Angel, K. Burdzy, and S. Sheffield. *Deterministic Approximations of Random Reflections*, arXiv:1203.0801v2, 2012.
- [2] G. Arya, H.-C. Chang, and E. J. Maginn. *Knudsen Diffusivity of a Hard Sphere in a Rough Slit Pore*, Physical Review Letters, 91, No. 2, July 2003, 026102(4).
- [3] H. Babovsky. *On Knudsen flows within thin tubes*, J. Stat. Phys., 44, Nos. 5/6, 865-878, 1986.
- [4] P.B. Bálint and S. Gouëzel, *Limit theorems in the stadium billiard*. Comm. Math. Phys. 263, 451-512, 2006.
- [5] P. Billingsley, *Convergence of Probability Measures*, John Wiley & Sons, New York, 1968.
- [6] C. Börgers, C. Greengard, and E. Thomann. *The diffusion limit of free molecular flow in thin plane channels*, SIAM J. Appl. Math. 52, No. 4, 1057-1075, 1992.
- [7] R.C. Bradley. *A Sufficient Condition for Linear Growth of Variances in a Stationary Random Sequence*, Proceedings of the American Mathematical Society, Vol. 83, No. 3 (Nov., 1981), pp. 586-589
- [8] C. Cercignani and D. H. Sattinger, *Scaling Limits and Models in Physical Processes*, DMV Seminar Band 28, Birkhäuser, 1998.
- [9] F. Celestini and F. Mortessagne, *Cosine law at the atomic scale: toward realistic simulations of Knudsen diffusion*, Physical Review E 77, 021202 (2008).
- [10] N. Chernov and R. Markarian, *Chaotic Billiards*, Mathematical Surveys and Monographs, 127, American Mathematical Society, 2006.
- [11] T. Chumley, S. Cook and R. Feres, *From billiards to thermodynamics*, 2012, arXiv:1207.5878v1
- [12] F. Comets, S. Popov, G. M. Schutz, M. Vachkovskaia, *Billiards in a general domain with random reflections*. Arch. Ration. Mech. Anal. 191 (2008), 497-537.
- [13] F. Comets, S. Popov, G. M. Schutz, M. Vachkovskaia, *Knudsen gas in a finite random tube: transport diffusion and first passage properties*, J. Stat. Phys. 140, 948-984 (2010).
- [14] S. Cook and R. Feres, *Random billiards with wall temperature and associated Markov chains*, Nonlinearity 25 (2012) 2503-2541.
- [15] R. Feres, *Random walks derived from billiards*, in Dynamics, Ergodic Theory, and Geometry, Ed. Boris Hasselblatt, MSRI Publications, Cambridge University Press, (2007) 179-222.

- [16] R. Feres and H-K. Zhang, *The spectrum of the billiard Laplacian of a family of random billiards*, Journal of Statistical Physics, V. 141, N. 6 (2010) 1030-1054.
- [17] R. Feres and H-K. Zhang, *Spectral Gap for a Class of Random Billiards*, Comm. Math. Phys. 313, 479-515, 2012.
- [18] R. Feres, J. Ng, and H-K. Zhang, *Multiple scattering in random mechanical systems and diffusion approximation*. (2012) <http://arxiv.org/abs/1208.3776>
- [19] S. Harris, *An introduction to the theory of the Boltzmann equation*, Dover, 1999.
- [20] C. Kipnis and S. R. S. Varadhan. *Central Limit Theorem for Additive Functionals of Reversible Markov Processes and Applications to Simple Exclusions*, Commun. Math. Phys. 104, 1-19, 1986.
- [21] P. E. Kloeden and E. Platen, *Numerical Solutions of Stochastic Differential Equations*, Springer, 1995.
- [22] G. Marin and G.S. Yablonsky. *Kinetics of Chemical Reactions*, Wiley-VCH, 2011.
- [23] S. Meyn and R. L. Tweedie, *Markov Chains and Stochastic Stability*, second edition, Cambridge University Press, 2009.
- [24] B. Oksendal, *Stochastic Differential Equations*, Springer, 1998.
- [25] D. W. Stroock, S. R. S. Varadhan, *Multidimensional Diffusion Processes*. Classics in Mathematics, Springer, 2006.
- [26] L. Tierney, *A note on Metropolis-Hastings kernels for general state spaces*. The Annals of Applied Probability (1998), Vol. 8, No. 1, 1-9.
- [27] J. Weidmann, *Linear operators in Hilbert spaces*. Springer-Verlag, New York 1980
- [28] W. Whitt . *Weak convergence of probability measures on the function space $C[0, \infty)$* . Ann. Math. Statist. 41 (1970) 939-944